SEVENTH FRAMEWORK PROGRAMME
Research Infrastructures

INFRA-2011-2.3.5 – Second Implementation Phase of the European High Performance Computing (HPC) service PRACE

PRACE-2IP

PRACE Second Implementation Project

Grant Agreement Number: RI-283493

D7.2.1
Technical Support for DECI Projects

Final

Version: 1.0
Author(s): Lilit Axner, SNIC-PDC
Date: 24.08.2012

Project and Deliverable Information Sheet

PRACE Project	**Project Ref. №: RI-283493**	
	Project Title: PRACE Second Implementation Project	
	Project Web Site: http://www.prace-project.eu	
	Deliverable ID: D7.2.1	
	Deliverable Nature: DOC_TYPE: Report	
	Deliverable Level: PU *	**Contractual Date of Delivery:** 31 / August / 2012
		Actual Date of Delivery: 31 / August / 2012
	EC Project Officer: Leonardo Flores Añover	

* - The dissemination level are indicated as follows: **PU** – Public, **PP** – Restricted to other participants (including the Commission Services), **RE** – Restricted to a group specified by the consortium (including the Commission Services). **CO** – Confidential, only for members of the consortium (including the Commission Services).

Document Control Sheet

Document	**Title: Technical Support for DECI Projects**	
	ID: D7.2.1	
	Version: 1.0	**Status:** ***Final*** *Final*
	Available at: http://www.prace-ri.eu	
	Software Tool: Microsoft Word 2007	
	File(s): D7.2.1.docx	
Authorship	**Written by:**	Lilit Axner, SNIC-PDC
	Contributors:	Wim Rijks (SARA) Isabelle Dupays (IDRIS) Petri Nikunen(CSC) Kai Brandhorst (FZJ) Nicole Audiffren (CINES) Michael Lysaght (ICHEC) Joachim Hein (SNIC-LUNARC) Luis Fazendeiro (SNIC-Chalmers) Christian Simarro (BSC) David Vicente (BSC) Jorge Rodriguez (BSC) Tilman Dannert (RZG) Alexander Block (LRZ) Xu Guo (EPCC) Chris Johnson (EPCC) Joerg Hertzer (HLRS) Andrew Emerson (CINECA) Giuffreda Maria Grazia (CSCS) Agnieszka Kwiecień (WCSS)
	Reviewed by:	Georgi Prangov, NCSA and Florian Berberich, FZJ
	Approved by:	MB/EB

Document Status Sheet

Version	Date	Status	Comments
0.1	6/June/2012	Draft	Initial draft
0.2	26/June/2012	Draft	With all the input
0.3	27/June/2012	Draft	Native speaker review
1.0	01/August/2012	Final version	Ready for PRACE review

Document Keywords

Keywords:	PRACE, HPC, Research Infrastructure, DECI, Enabling, Technical Evaluation, Scalability, Performance

Table of Contents

List of Figures

List of Tables

References and Applicable Documents

[1] http://www.prace-ri.eu
[2] D4.3.2 The 3.2 Cross-national Programme for Tier-1 Access Pilots (PRACE-1IP deliverable)
[3] D4.3.1 Cross-national programme for access to Tier-1 resources (PRACE-1IP deliverable)
[4] D2.1 Migration from DEISA2 to PRACE-2IP (PRACE-2IP deliverable)

PRACE public deliverables can be found on the PRACE Web site at http://www.prace-ri.eu/Public-Deliverables#PD_1IP and http://www.prace-ri.eu/Public-Deliverables#PD_2IP respectively.

List of Acronyms and Abbreviations

AMD	Advanced Micro Devices
API	Application Programming Interface
BAdW	Bayerischen Akademie der Wissenschaften (Germany)
BLAS	Basic Linear Algebra Subprograms
BSC	Barcelona Supercomputing Center (Spain)
BSCW	Be Smart Cooperate Worldwide public cooperation platform on the Internet
CEA	Commissariat à l'Energie Atomique et aux énergies alternatives (represented in PRACE by GENCI, France)
CINECA	Consorzio Interuniversitario, the largest Italian computing centre (Italy)
CINES	Centre Informatique National de l'Enseignement Supérieur (represented in PRACE by GENCI, France)
CLE	Cray Linux Environment
CPU	Central Processing Unit
CSC	Finnish IT Centre for Science (Finland)
CSCS	The Swiss National Supercomputing Centre (represented in PRACE by ETHZ, Switzerland)
CUDA	Compute Unified Device Architecture (NVIDIA)
DECI	Distributed Extreme Computing Initiative
DEISA	Distributed European Infrastructure for Supercomputing Applications. EU project by leading national HPC centres.
DP	Double Precision, usually 64-bit floating point numbers
DPMDB	DECI Process Management DataBase
EC	European Community
EESI	European Exascale Software Initiative
EoI	Expression of Interest
EPCC	Edinburg Parallel Computing Centre (represented in PRACE by EPSRC, United Kingdom)
EPSRC	The Engineering and Physical Sciences Research Council (United Kingdom)
ETHZ	Eidgenössische Technische Hochschule Zuerich, ETH Zurich (Switzerland)
ESFRI	European Strategy Forum on Research Infrastructures; created roadmap for pan-European Research Infrastructure.
FFT	Fast Fourier Transform
FHPCA	FPGA HPC Alliance
FP	Floating-Point
FPGA	Field Programmable Gate Array

FPU	Floating-Point Unit
FZJ	Forschungszentrum Jülich (Germany)
GB	Giga (= 2^{30} ~ 10^9) Bytes (= 8 bits), also GByte
Gb/s	Giga (= 10^9) bits per second, also Gbit/s
GB/s	Giga (= 10^9) Bytes (= 8 bits) per second, also GByte/s
GCS	Gauss Centre for Supercomputing (Germany)
GÉANT	Collaboration between National Research and Education Networks to build a multi-gigabit pan-European network, managed by DANTE. GÉANT2 is the follow-up as of 2004.
GENCI	Grand Equipement National de Calcul Intensif (France)
GFlop/s	Giga (= 10^9) Floating point operations (usually in 64-bit, i.e. DP) per second, also GF/s
GHz	Giga (= 10^9) Hertz, frequency =10^9 periods or clock cycles per second
GigE	Gigabit Ethernet, also GbE
GLSL	OpenGL Shading Language
GNU	GNU's not Unix, a free OS
GPGPU	General Purpose GPU
GPU	Graphic Processing Unit
HET	High Performance Computing in Europe Taskforce. Taskforce by representatives from European HPC community to shape the European HPC Research Infrastructure. Produced the scientific case and valuable groundwork for the PRACE project.
HP	Hewlett-Packard
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
IB	InfiniBand
IBM	Formerly known as International Business Machines
IDRIS	Institut du Développement et des Ressources en Informatique Scientifique (represented in PRACE by GENCI, France)
IEEE	Institute of Electrical and Electronic Engineers
IESP	International Exascale Project
I/O	Input/Output
ISC	International Supercomputing Conference; European equivalent to the US based SC0x conference. Held annually in Germany.
JSC	Jülich Supercomputing Centre (FZJ, Germany)
KB	Kilo (= 2^{10} ~10^3) Bytes (= 8 bits), also KByte
KTH	Kungliga Tekniska Högskolan (represented in PRACE by SNIC, Sweden)
LINPACK	Software library for Linear Algebra
LRZ	Leibniz Supercomputing Centre (Garching, Germany)
MB	Mega (= 2^{20} ~ 10^6) Bytes (= 8 bits), also MByte
MB/s	Mega (= 10^6) Bytes (= 8 bits) per second, also MByte/s
MFlop/s	Mega (= 10^6) Floating point operations (usually in 64-bit, i.e. DP) per second, also MF/s
MHz	Mega (= 10^6) Hertz, frequency =10^6 periods or clock cycles per second
Mop/s	Mega (= 10^6) operations per second (usually integer or logic operations)
MoU	Memorandum of Understanding.
MPI	Message Passing Interface
MPP	Massively Parallel Processing (or Processor)
MPT	Message Passing Toolkit
NUMA	Non-Uniform Memory Access or Architecture
OpenCL	Open Computing Language

OpenGL	Open Graphic Library
Open MP	Open Multi-Processing
OS	Operating System
PDC	HPC centre at KTH
PGAS	Partitioned Global Address Space
PGI	Portland Group, Inc.
PI	Principal Investigator
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PSNC	Poznan Supercomputing and Networking Centre (Poland)
RAM	Random Access Memory
RDMA	Remote Data Memory Access
SARA	Stichting Academisch Rekencentrum Amsterdam (Netherlands)
SE	Scientific Evaluation
SGI	Silicon Graphics, Inc.
SMP	Symmetric MultiProcessing
SNIC	Swedish National Infrastructure for Computing (Sweden)
SP	Single Precision, usually 32-bit floating point numbers
STFC	Science and Technology Facilities Council (represented in PRACE by EPSRC, United Kingdom)
STRATOS	PRACE advisory group for STRAtegic TechnOlogieS
TB	Tera (= 240 ~ 1012) Bytes (= 8 bits), also TByte
TE	Technical Evaluation
TFlop/s	Tera (= 1012) Floating-point operations (usually in 64-bit, i.e. DP) per second, also TF/s
Tier-0	Denotes the apex of a conceptual pyramid of HPC systems. In this context the Supercomputing Research Infrastructure would host the Tier-0 systems; national or topical HPC centres would constitute Tier-1
UYBHM	National Center for High Performance Computing of Turkey

Executive Summary

This deliverable reports on technical support for DECI (Distributed European Computing Initiative) projects in the first year of the PRACE-2IP project. During this period three DECI calls were launched: DECI7 (pilot call), DECI8 and DECI9. As a result 35 DECI7 projects and 33 DECI8 projects were accepted and have already started their runs and made progress successfully on assigned PRACE systems, while the applications for the DECI9 call are in the process of scientific evaluation. PRACE experts engaged in T7.2 of WP7 continuously help the users of DECI7 and DECI8 projects to run their codes on the assigned PRACE systems. 15 out of 35 DECI7 and 13 out of 33 DECI8 projects requested enabling help for their projects going beyond the usual assistance in getting access and porting the code to the execution platform. This requires an engagement of T7.2 PRACE experts for up of 6 months in optimizing and/or scaling the given code. This work has been successfully accomplished for DECI7 projects that will finish their runs by the end of October 2012, however T7.2 continues to keep track of the progress of DECI7 projects and to offer help if the need arises. The work on DECI8 projects is ongoing as the allocation period will persist until May 2013. The enabling work on DECI9 projects will start from November 2012. T7.2 is not only responsible for enabling but also for the technical evaluation of DECI applications. The technical evaluations of all DECI7, DECI8 and DECI9 applications have already been successfully completed. The results of these technical evaluations have been communicated to the scientific evaluation committees and have been taken into account in the final selection process.

The whole work process of T7.2 is in close cooperation with T2.2 of WP2 and with WP6 of the PRACE-2IP project.

1 Introduction

Starting from the PRACE-2IP project a follow-up activity to the successful DECI (DEISA Extreme Computing Initiative) was initiated. This activity allows researchers to access significant amounts of time on Tier-1 systems in different European countries. Task 7.2 provides technical input to the selection process of these projects. After the selection process, T7.2 provides optimisation and scaling support for the successful proposals in collaboration with the users and the developers of the relevant application codes. This document reports on the progress during the first PRACE-2IP project year as well as describing the future plans for the second project year.

Section 1 gives an introduction to this document, its structure and describes the main objectives of the task.

Section 2 gives an overview of the available task force for this task as well as highlighting the relationship between WP7-T7.2, WP2-T2.2 and WP6 of PRACE-2IP project.

Section 3 gives an overview of the DECI7 call and describes the enabling work for the projects requesting it.

Section 4 gives an overview of the DECI8 call and describes the enabling work for the projects requesting it.

Section 5 gives an overview of the DECI9 call.

Section 6 summarizes the progress of the year and outlines the future work in reference to all DECI calls.The document is intended for public audience and describes the enabling work done in this task in detail including references to the other related work packages.

2 Overview of the Task - Applications Support for new DECI Projects

The task of giving technical support to DECI applications consists of two stages:

- technical evaluations of DECI incoming applications
- help with enabling of accepted projects on DECI Tier-1 systems.

After the closing date of each DECI call the submitted proposals are collected by WP2 in a dedicated folder on BSCW. Afterwards the staff members of T7.2 perform the technical evaluation of these projects, using a template form, specially developed for this purpose. The technical evaluations are completed within two weeks and uploaded to BSCW as well. The next stage is the scientific evaluation of the proposals, which falls under the responsibility of WP2. WP7-T7.2 has no responsibility for this part. However, after scientific evaluation, when the list of accepted proposals is known, T7.2 resumes its activities of enabling the projects of these accepted proposals on their assigned Tier-1 systems. The enabling work is diverse and ranges from making sure that the investigator can successfully log on to the execution site to comprehensive help with the scalability and performance work on the code itself.

All these activities within T7.2 are being monitored by monthly teleconferences and the progress is reported on a dedicated web portal where the workflow for each project is logged. Finally this deliverable as well as deliverable D7.2.2 at the end of August 2013 reports in detail all the work done in T7.2 task on all DECI projects.

2.1 Technical Evaluation Procedure of DECI applications

As was described in deliverable D2.1 (see [4]), WP2, the technical evaluation (TE) has to be completed within two weeks after the closing date of the corresponding DECI call. The Technical reviews are currently distributed across PRACE partners participating in DECI. Each partner reviews the proposals originating from PIs of their own country. This partner is appointed as the proposal's home site. Exceptions to this rule are countries that do not participate in PRACE and proposals that need collaboration between several DECI partners. In these cases proposals are assigned based on geographical proximity of applicants, former contacts with them, and the number of proposals assigned to the sites (to balance effort). This process is illustrated in Figure 1.

Technical evaluation (TE) is currently based on a Word document form that was used in the DEISA DECI process, but adapted to the altered layout of the DECI-7 proposal form. The completed TEs are uploaded to the PRACE BSCW by T7.2 members. These TEs together with the project proposals are sent to the peer review committees by WP2 representatives. In parallel to this T7.2 staff populate the DPMDB (DECI Process Management DataBase) with the applications' technical information to be used in future DECI activities by WP2 and WP6 of the PRACE-2IP project.

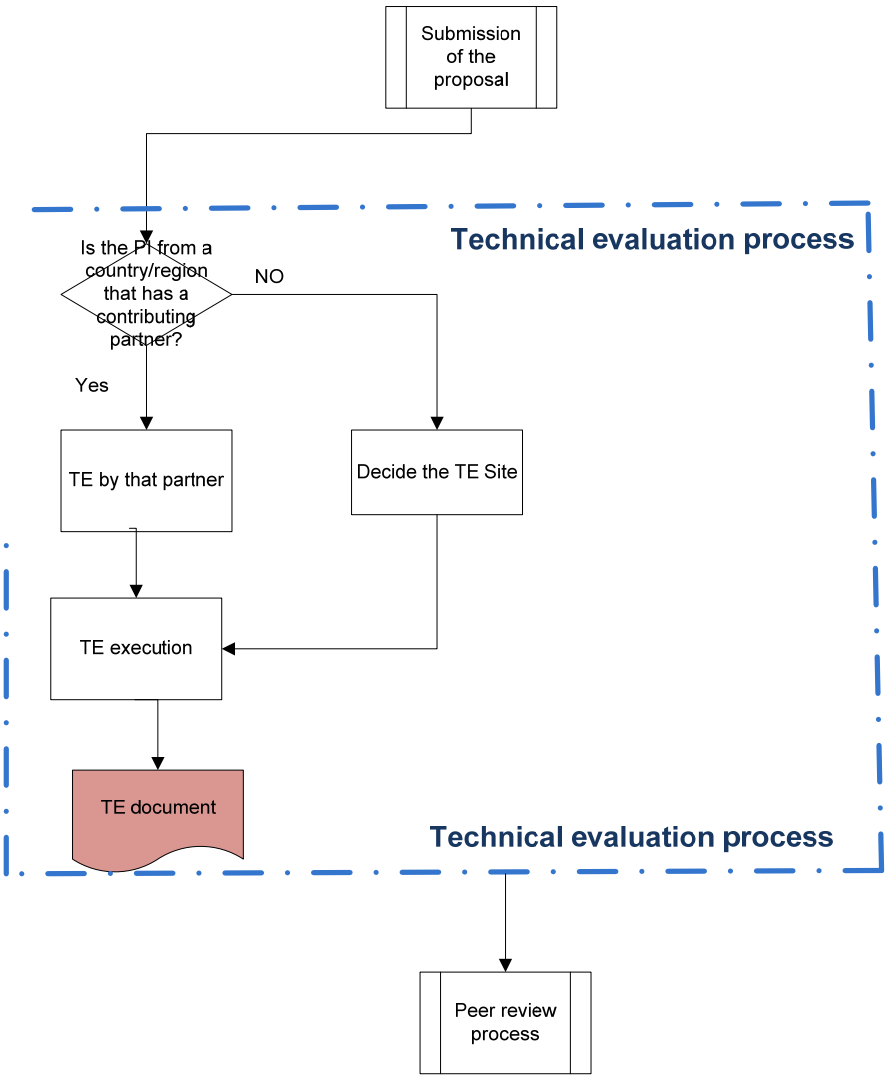


Figure 1: Technical evaluation process (figure taken from D4.3.2 of the PRACE-1IP project)

TEs are usually done in close communication with PIs as a lot of technical details need to be clarified for the best choice of assigned system. Currently for each DECI call over 15 systems throughout Europe can be available and thus choosing the most appropriate system is far from trivial. A detailed TE is therefore very important and is one of the main reasons why the TEs are done by the proposal's home site that has closest contact with the PI and may also be well acquainted with the code.

It is also worth mentioning that the use of Word document format for not only the TE, but also the scientific evaluation (SE) and project application forms, is extremely inconvenient since during the evaluation procedures T7.2 members have to copy and paste a lot of information from one form to another. The solution to this problem would be the implementation of a web based DECI Submission and Evaluation tool to facilitate efficient and centralized control and supervision of the TE process. Similar tools have already been implemented in other projects such as HPC Europa as well as for the Tier-0 access within PRACE. Currently a small team with members from WP2 and T7.2 are evaluating these tools with the aim at recommending one of them for the implementation of the DECI Submission and Evaluation tool. It should be emphasised though that there are several fundamental differences between these tools and a thorough examination and discussion are necessary.

2.2 Enabling support of Accepted Applications

In D4.3.1 (see [3]) of the PRACE-1IP project it has been reported and confirmed by questionnaire that application support within DECI aims to facilitate a better understanding of the likely requirements of future users of the Tier-0 systems by collecting real use-case information about the needs and capabilities of scientific codes and about the differences between usage of national and European resources and facilities. By working on scalability and performance aspects of scientific codes, application support enables DECI to become a very effective instrument for providing a ramp from Tier-1 to Tier-0.

Moreover, the possibility of having applications experts from leading European HPC centres provide support to scientists that are interested in using the opportunity within DECI to experiment with new architectures is also highly valued.

Within the PRACE-2IP project application support is a responsibility of WP7 task 7.2. Application experts from each DECI site and from other PRACE HPC centres that are not active in DECI but have expressed their wish to assist DECI applicants have been identified for this task.

T7.2 assigns each DECI accepted project an expert from the home site (the site that helped the applicant to apply for DECI call) as well as an expert from the execution site (the site where the application is going to be executed). If the DECI application has multiple execution sites then an expert from each execution site assigned to help with porting of the code to the given system.

The application expert from the home site has the following obligations:

1. Contact the PI (either by physically visiting him/her or by phone or finally by email if PI is an experienced DECI user from a previous DECI call). During the meeting the home site expert should explain the whole DECI procedure from the user point of view, provide information about the assigned execution site and remind the user of the necessity for submitting a report at the end of the project The home site expert should also assist the PI with obtaining a national x.509 certificate that is highly recommended for acquiring access to the PRACE infrastructure.
2. Assure that the execution site expert is informed about the PI and has necessary information to help the PI to port the code to the execution system.

It is important to note that the home site expert is responsible for informing the PI about the services PRACE provides including:

- The PRACE helpdesk and contact information
- Module environment
- PRACE common work environment
- PRACE user documentation

The execution site expert helps with porting of the code to the assigned machine.

As well as home site and execution site experts, T7.2 also assigns one expert, called the enabling expert, to projects that have indicated in the DECI application form that they needed elaborate help with their codes. The home site expert, the execution site expert or an expert from a third DECI site can be appointed as enabling expert who has a major and very important task to work with the PI in an intensive manner to help with:

- performance
- scalability
- optimization
- parallelization aspects of the code.

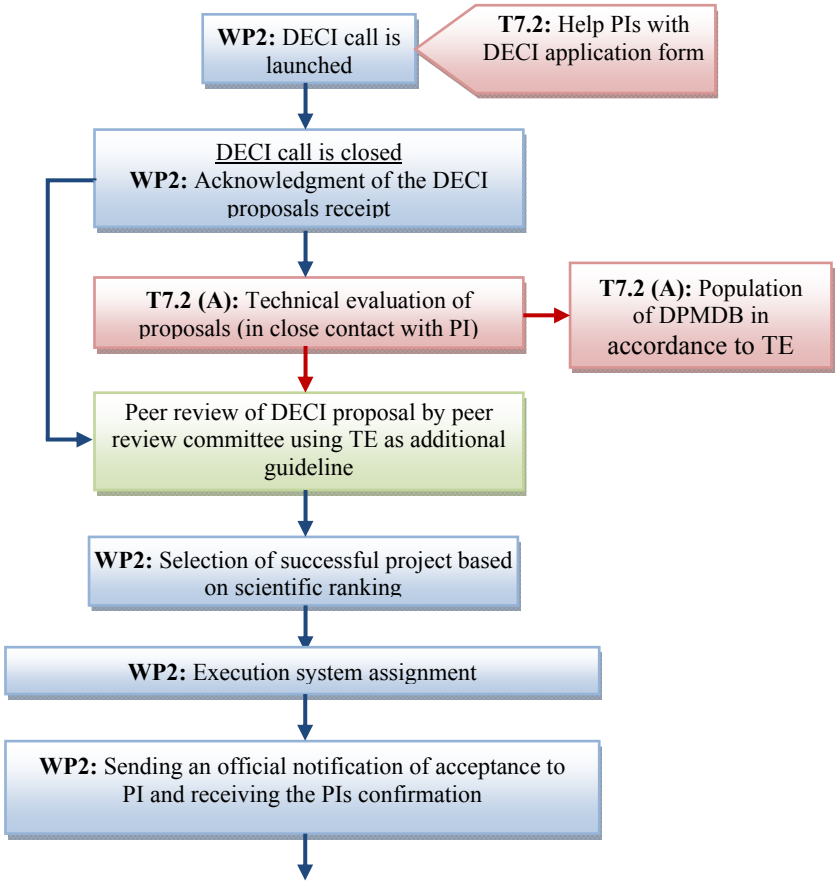
The amount of effort and the timeframe for this enabling task is being estimated for each DECI application separately during the technical review of the proposal. The timeframe may vary between 1 to 6 months depending on the PI's specified request.

As soon as the PI has access to the assigned execution system, the enabling expert contacts the PI and starts the work on the code. The progress of this work is logged in a dedicated workflow database and can be easily followed by all members of the T7.2 task.

Whether or not the PI requested enabling the execution of the project should start as soon as possible and the progress should be constantly monitored.

2.3 Relationship with Other Work Packages

As shown in Figure 2 there is a very close collaboration between WP7-T7.2, WP2-T2.2 and WP6 of PRACE-2IP project during the whole DECI process. All three are essential in the DECI infrastructure.



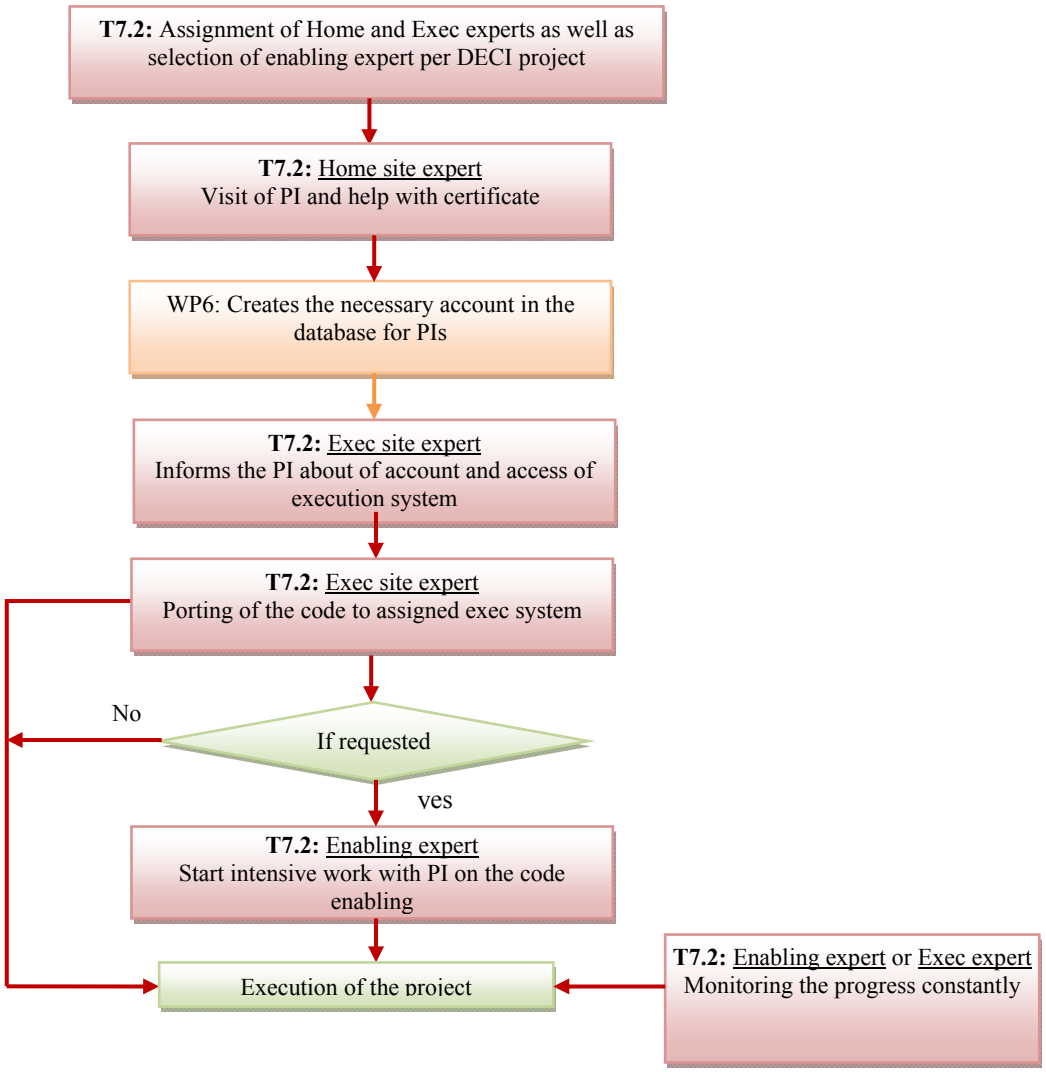


Figure 2:The DECI process

While WP2 prepares the DECI call, collects the proposals and coordinates the whole DECI process from start to an end, T7.2 has the closest contact with PIs and helps them throughout the whole DECI year. WP6 on the other hand ensures that the common environment on all DECI systems is ready, functioning and accounts are ready for the PIs to smoothly log into the systems and run their codes. Thus it is crucial to maintain a constant up to date information flow between these three parties.

2.4 Available Workforce

The activities within T7.2 of the PRACE-2IP project started quite early in September 2011 with the enabling work of pilot DECI7 projects. In the beginning of the process the task leader collected the complete list of experts from all PRACE sites that are active in T7.2. The T7.2 experts joined the T7.2 dedicated mailing list and informed the task leader about available project months (PMs) that they were intending to dedicate to this application support work. In total around 180PMs from 24 partners are available in the task.

However one needs to differentiate between partners that are active in a given DECI call and the partners that have dedicated efforts in T7.2. Irrespective of whether a PRACE partner has

committed resources to a specific DECI call, it still may be active in task T7.2 and provide application support to DECI projects.

At the moment of writing this deliverable, the projects of the two DECI calls, DECI7 and DECI8, are in the stage of production runs. For each of these two calls about 40PMs of help with enabling was asked for by the projects, however the actual enabling effort is still to be revaluated at the end of the access periods after the enabling work is finished on all projects. The results of the DECI9 call will be known in October/November 2012. Considering this estimate, T7.2 has sufficient personnel to help PIs with their DECI projects.

2.5 Tools in Use

The progress of the DECI projects is monitored by their home sites, and the status is recorded in the DPMDB. The status of the enabling activity is recorded in the Best Practice Workflow. A snapshot of this tool is depicted in Figure 3.

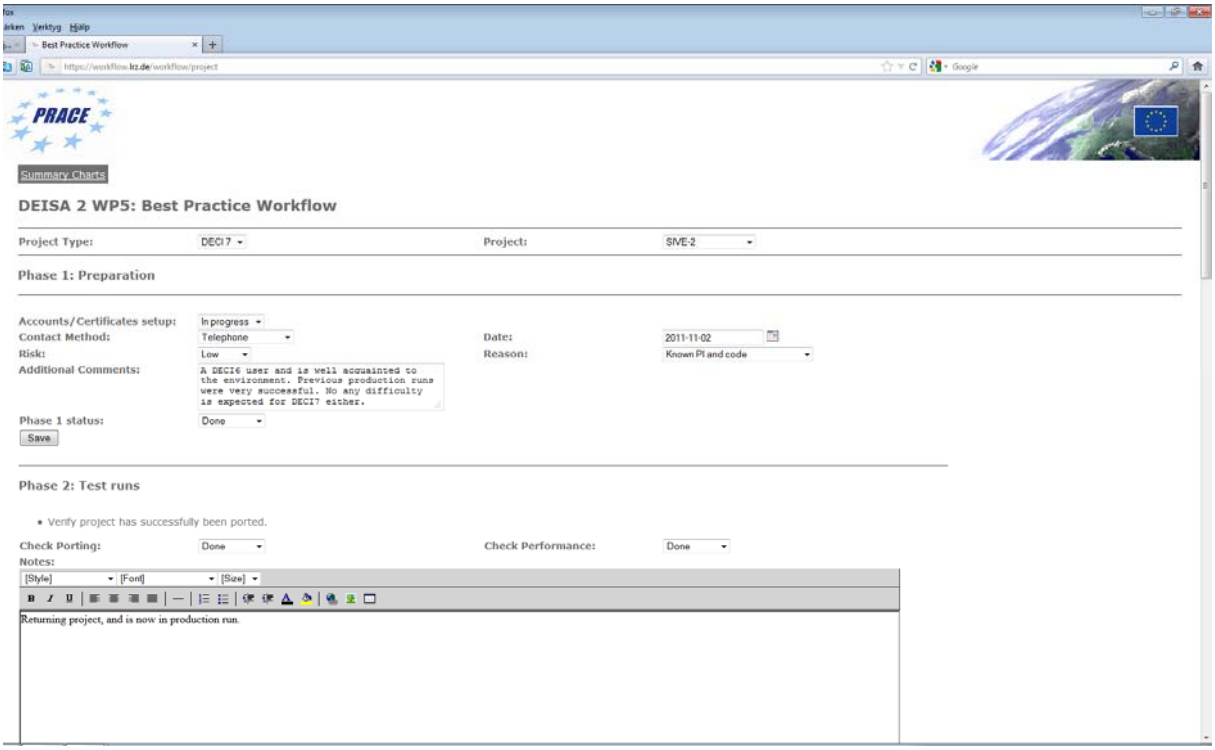


Figure 3: DECI workflow tool

The information in this tool is updated periodically and the progress is reported during the monthly T7.2 teleconferences. The tool is hosted by the PRACE partner LRZ and access is granted based on certificate identity. This tool has been developed and been extensively used previously in the DEISA project.

Another tool that is used to monitor the progress of DECI projects is DPMDB. This tool is mainly used by T2.2 to monitor the progress of used vs. granted CPU hours per project. The DPMDB is updated by extracting the usage per project from another central accounting tool called DART or provided by the execution site expert if the site is not connected to DART. Detailed information on this has been reported in PRACE-2IP deliverable D2.1 [4].

3 Enabling Work on DECI7 Projects

The DECI7 call was a pilot call parallel with the 3rd PRACE call for Tier-0 applications. It was launched on 2nd of May 2011 and closed on 22nd of June 2011. Thus this call was announced before the PRACE-2IP project started. The access and consequently the application support for the DECI7 accepted projects started from 1st of November 2011.

As mentioned above T7.2 started from September 2011 by collecting the information about active partners in this task. These preparatory activities ensured a smooth start of the work on DECI7 accepted projects.

As a result 35 DECI7 proposals have been accepted of which about six requested substantial support (between 2 to 6 months of work) for enabling of these codes. The list of this projects as well as the requested support is listed in Table 1.

Home site	Project	Execution site(s)	Enabling PMs
BSC	BlackHoles	PSNC	0,5
BSC	CatDesign	LRZ, PSNC	0,5
CINECA	MAESTRO	IDRIS	0,5
CINECA	MIXTUDI	FZJ, CINECA	0,5
CINECA	PETAHUB	NCSA, SNIC-PDC	0,5
CINECA	SCW	LRZ	1,0
CINES	ElmerIce	SNIC-PDC	3 to 6
CINES	NUWCLAY	CINECA	0,5
CSC	Planck-LFI	CSC	1 to 3
CSC	TanGrin	EPCC	0,5
CSCS (HLRS)	VIRonSAMs	CINES, CINECA	0,5 to 1
EPCC	EC4aPDEs-2	BSC, CSC, HLRS, IDRIS	0,5
EPCC	HELIXKINETICS	ICHEC, FZJ	0,5
EPCC	HIFLY	PSNC	0,5
EPCC	HYDROGEN-ILs	SNIC-PDC	0,5
FZJ	HIGHQ2FF	SNIC-PDC	0,5
FZJ	NR-NSNS-BHNS	CSC	1,0
HLRS	DIAVIB	CINECA, SARA	0,5
HLRS	PHOTMAT	PSNC, CINES	0,5 to 1

ICHEC	LGICTAMD	ICHEC	0,5
ICHEC	NANOBIO-2	HLRS, CINES	0,5
IDRIS	PICKH	CINECA	3,0
IDRIS	WESF	RZG, CSC	0,5
LRZ	CASiMIR	SARA	0,5
PSNC	SIMONA	SARA, PSNC, IDRIS	0,5 to 1
RZG	ARTHUS-3	FZJ	0,5
RZG	EUTERPE-4	FZJ	0,5
RZG	LASIPROD	LRZ	1,0
RZG	SMARC	LRZ	0,5
SARA	HRPIPE	SNIC-PDC	0,5
SARA	RBflow-2	RZG, SARA	0,5
SNIC-PDC	DiSMuN	SNIC-PDC, SARA	2,0
SNIC-PDC	MUSIC	IDRIS	2,0
SNIC-PDC	SIVE-2	EPCC	0,5
SNIC-PDC	SPIESM	SNIC-PDC	2,0

Table 1: Enabling effort requests of DECI7 projects with home and execution sites.

Table 2 lists the same DECI7 projects per architecture.

Architecture	**DECI7 Projects**
IBM BG/P	MAESTRO, PETAHUB, WESF, MUSIC
IBM Power 6	PICKH, DIAVIB, NUWCLAY, CASiMIR, SIMONA, RBflow-2, DiSMuN, MIXTUDI
CRAY (XT4/5, XE6)	ElmerIce, TanGrin, HYDROGEN-ILs, HIGHQ2FF, DiSMuN, SIVE-2, HRPIPE, SPIESM, Planck-LFI, NR-NSNS-BHNS
Clusters (SuperMUC migration, Bull Nehalem, NEC Nehalem, SGI ICE E8200, SGI UV1000, HP)	VIRonSAMs, EC4aPDEs-2, HIFLY, MIXTUDI, ARTHUS-3, EUTERPE-4, NANOBIO-2, HELIXKINETICS, LGICTAMD, BlackHoles, PHOTMAT, CatDesign, SCW, SMARC, LASIPROD

Table 2: DECI7 projects per architecture

Table 3 lists the DECI7 projects per discipline.

Discipline	DECI7 Projects
Astro Sciences	ARTHUS-3, BlackHoles, MAESTRO, PICKH, Planck-LFI, SMARC
Bio Sciences	HELIXKINETICS, LASIPROD, LGICTAMD, MUSIC, SIVE-2, TanGrin, VIRonSAMs
Earth Sciences	CASiMIR, ElmerIce, SPIESM
Engineering	HIFLY, HRPIPE, MIXTUDI, RBflow-2, WESF
Materials Science	CatDesign, DIAVIB, DiSMuN, EC4aPDEs-2, HYDROGEN-ILs, NANOBIO-2, NUWCLAY, PETAHUB, PHOTMAT, SCW, SIMONA
Plasma & Particle Physics	EUTERPE-4, HIGHQ2FF

Table 3: DECI7 projects per discipline

The application support for the projects can involve different tasks and levels. For some projects experts may also encounter some unexpected difficulties. For this reason the details of the application support work for each project are listed below. The project status indicates the amount of CPU hours used in relation to the granted amount of CPU hours expressed as a percentage.

Project Acronym: BlackHoles

Source of Project: DECI-7 (2011-2012)

PRACE Home site: BSC

PRACE Enabling sites: BSC, PSNC

PRACE Execution site: PSNC

PRACE Architectures: SGI UV1000

Start enabling: March2012

Start production: April 2012

Project status: In progress (2%)

Description of project:

Black holes dynamics in metric theories of gravity is an Astrophysics project led by Dr. Vitor Cardoso. Numerical modelling of Black Holes in non-asymptotically flat spacetimes in metric theories of gravity, including GR, is still in its infancy and here they propose to extend their previous studies to BHs in spacetimes with a non-zero cosmological constant. Imprints of alternative theories are most likely to be carried by the Gravitational Waves generated in highly dynamical processes involving black holes, and will become observable in the next decade by the several operating detectors worldwide.

Types of work undertaken:

The LDAP accounts for the project were created. However the production of the SGI-Altix UV 1000 machine at PSNC was delayed. In order to speed up the enabling process and to be ready to start production runs as soon as the PSNC machine was in production, BSC proposed that the PI to compile their code on the SGI-Altix machine at BSC. BSC solved some problems in the code and made scalability test runs on their machine.
As the problems with the SGI-Altix continued at PSNC, BSC decided together with PSNC to move the project to the AMD-GPU cluster of PSNC instead. Once the PI‘s code was finally deployed on this cluster, BSC found some problems with the queue system at PSNC and MPI libraries that were fixed in collaboration with PSNC.

Difficulties encountered:

The project has only one execution site - PSNC. They encountered problems because the PSNC Tier-1 machine was not in production until March 23rd. Afterwards the machine was very unstable and the PIs were not able to start production runs. The instabilities did not disappear and PSNC proposed to use the CPUs of their GPU machine instead. The PIs were able to finally make production runs on this cluster. Because of these delays PSNC agreed to extend the activity consumption until March 2013.

Project Acronym: CatDessign

Source of Project: DECI-7 (2011-2012)

PRACE Home site: BSC

PRACE Enabling sites: BSC, SPNC

PRACE Execution site: LRZ, PSNC

PRACE Architectures: SuperMig, SGI UV1000

Start enabling: March 2012

Start production: March 2012

Project status: In progress (40%)

Description of project:

CatDesign is a Material Sciences project lead by Dr Ganduglia-Pirovano, Maria. The aim of the project is to elucidate the structure and functioning of Ni/CeO2 catalysts and to develop a molecular-level model for the Water Gas Shift reaction on such promising systems, which are currently under investigation by the experimental collaborators at both the Institute of Catalysis and Petrochemistry-CSIC in Madrid and the Brookhaven National Laboratory in the US. To this end they propose to create computational models for these catalysts and to apply density functional theory (DFT) based approaches, as implemented in the VASP code, to investigate atomic structures as well as electronic and chemical properties.

Types of work undertaken:

The LDAP accounts were created and PIs were able to start production runs at LRZ instantaneously since VASP was already installed and tested there. BSC contacted LRZ support to give the code license of the PI. The project has faced problems at PSNC, the second execution site. PIs had to wait until the machine at PSNC came into production later than expected. BSC installed VASP on the PSNC SGI-Altix machine since it was not installed previously. However, the SGI instabilities did not allow BSC to start the tests on time, so project was switched to AMD-GPU cluster at PSNC. BSC installed and tested VASP there because it was not installed on this machine either. The CatDesign members have not

been able to start to execute VASP at PSNC because of the lack of manpower on the PI side. They are still consuming hours at LRZ.

Difficulties encountered:

Many of the difficulties encountered were related to the SGI machine at PSNC. BSC also faced a couple of difficulties to compile VASP related to third-party libraries. The researcher in charge of the executions at PSNC is presently in China, which will add further delay to performing the production runs on that machine.

Project Acronym: MAESTRO

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CINECA

PRACE Enabling sites: IDRIS

PRACE Execution site: IDRIS

PRACE Architectures: BG/P

Start enabling: February 2012

Start production: March 2012

Project status: In progress (28%)

Description of project:

Collimated jets of ionized plasma are a common phenomenon observed in many astrophysical systems, from newly forming stars similar to Sun, where Herbig-Haro (HH) jets take their origin, X-Ray binaries, in which galactic microquasars are produced, or Active Galactic Nuclei (AGN), where relativistic jets associated with extended radio-galaxies are accelerated. The three dimensional simulations will represent the first attempt to globally model the launching mechanism of jets from magnetized Keplerian disks. The main aim is to study the stability of the accretion-ejection process and of the jet initial propagation to the onset of non-axisymmetric modes of instability.

Types of work undertaken:

Account creation and access to BG/P of Idris.

Difficulties encountered: None

Project Acronym: MIXTUDI

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CINECA

PRACE Enabling sites: CINECA, FZJ

PRACE Execution site: CINECA, FZJ

PRACE Architectures: Juropa Intel Cluster

Start enabling: November 2011

Start production: December 2011

Project status: In progress (43%)

Description of project:

In this project PIs propose to study systematically the mixing of a fluid in a fully developed turbulent channel flow. In particular, the project will focus on the connection between mixing processes and turbulence structures with specific focus on the coupling between turbulence and mass transport properties. This task will be achieved by means of high resolution pseudo-spectral of the CHNS system in turbulent channel flow. Different values of the Reynolds number (Re) will be considered, which measures turbulence intensity, of the Weber number (We) which measures the relative importance of fluid surface tension effects with respect to the inertial forces and of the Peclet number (Pe) which measures the relative importance of the fluid diffusivity properties. This study is expected to advance the state of the art in turbulent mixing simulations introducing an accurate and robust framework specifically tailored for this kind of analysis.

Types of work undertaken:

Account creation and help with interactive access.

Difficulties encountered: None.

Project Acronym: PETAHUB

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CINECA

PRACE Enabling sites: CINECA, SNIC-PDC, NCSA

PRACE Execution site: SNIC-PDC, NCSA

PRACE Architectures: CRAY XE6, BG/P

Start enabling: January 2012

Start production: June 2012

Project status: In progress (7%)

Description of project:

In this project PIs propose to study the phase diagram of the Hubbard model in two, dimensional lattices by using a highly developed quantum Monte Carlo method. The main purpose is to use the large computer power available by the PRACE call to obtain reliable simulations of the model on lattice sizes containing several hundred electrons

Types of work undertaken: Account creation

Difficulties encountered: None

Project Acronym: SCW

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CINECA

PRACE Enabling sites: CINECA, LRZ

PRACE Execution site: LRZ

PRACE Architectures: Intel Westmere EX@2.4

Start enabling: November 2012

Start production: December 2012

Project status: In progress (99%)

Description of project:

This project aims to study the behaviour of supercritical water (SCW) as a function of the system density, by means of *ab initio* Molecular Dynamics simulations. The proposers have just developed a new method to apply the force matching algorithm to polarizable models. The method yields electron cloud fluctuations in good agreement with *ab initio* ones, which is not possible with present empirical potentials. Eventually, two major outcomes of this study are expected: the first concerns the study of short time dynamics with first principles Molecular Dynamics (which, in itself, constitutes an important novelty in the field) and the second concerns the possibility of producing a new force field targeting the properties of SCW.

Types of work undertaken:

The performance and parallel scaling of the CP2K code used in the project on SuperMig was checked by running the same input on an installation of the program on CINECA's PLX cluster. The PLX version showed demonstrably higher performance and scaling, despite the fact that the architectural differences between the two clusters should be limited (with the exception of the GPUs). With this information a more recent version of the code was re-compiled on SuperMIG and performance is now being tested.

Difficulties encountered: None

Project Acronym: ElmerIce

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CINES

PRACE Enabling sites: CINES, CSC

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: November 2011

Start production: February 2012

Project status: In progress (40%)

Description of project:

This project uses the Elmer finite element modelling software with the Ice solver to provide accurate and reliable estimates on the future contribution of glaciers and ice sheets to sea-level rise.

Types of work undertaken:

The application used in the project was ported to SNIC-PDC's Cray XE6 system by CSC. The main issue in connection with a compilation of Elmer on the Cray is that Compute Node Linux by default does not support shared objects. Elmer, on the other hand, has a modular structure and hence depends on shared objects. Additionally, the main parallel sparse matrix solver libraries, Hypre and MUMPS (itself dependent on ScaLapack and BLACS) have to be compiled with particle independent code (using the -fPIC flag in common compiler suites).

The other important task done by CSC was the optimisation of algorithms for discrete saddle point systems in Elmer. The Elmer/Ice applications bring along the fact that the Stokes equations have to be solved in connection with a strong non-linear power law rheology (Norton–Hoff law, Glen's flow law in glaciology). With the preconditioners traditionally available (basically ILU), in most real geometries it was very difficult, if not impossible, to achieve convergence of the linear system with memory and cycle-effective iterative Krylov subspace methods. The only available parallel direct solution method, MUMPS, on the other hand is memory intensive and limited in its scalability. In fact, it would have been better suited to a machine with more memory per core than the Cray.

The only real alternative to MUMPS is to apply Krylov methods in combination with preconditioning strategies that are designed specially for handling discrete saddle point problems. In particular, CSC were developing a block preconditioner which is derived from a field-wise split of the discrete system into equations characterizing the velocity and pressure variables. In this way, the action of the preconditioner may be computed by performing approximate solves of sub-problems that with a specific scaling are solvable in a much easier and compact way. In order to be able to deploy the block preconditioner, the following particular points have been addressed:

- As the preconditioned solver was found to perform well also for systems arising from the Newton linearization, the nonlinear solution process can now be accelerated significantly even in connection with the effective preconditioning.
- Linear system scaling strategies to improve the condition number of systems that need to be handled were optimised. Linear system scaling can now be done separately for the primary linear system and for the preconditioning systems, so that the effects of ill-conditioning are reduced in all phases of computation.
- To enable a flexible way to improve finite element stability, the finite element approximation utilises bubble functions of the p-version of the finite element method. The stability and the ability of the preconditioned solver to handle realistic cases with high element aspect ratios have been verified experimentally.
- The performance tests indicate that the preconditioner performance is now nearly independent of the problem size if the element aspect ratio remains the same. The performance anyhow depends critically on the efficiency of subsidiary computations to obtain the velocity updates. Further splitting strategies to solve velocity components independently have been explored in order to enable the full scalability of the solution procedure.

The research group is currently conducting benchmark runs on the Cray to elaborate the different numerical parameters and solution strategies of the subproblems in order to optimise the performance with the constraint of the robustness.

Difficulties encountered:

In the proposal, the type of simulations were clearly described as long simulations (200 hours) requiring ten's to hundred cores (<256) and quite a large memory per core (1 to 2 Go/core). Clearly, Cray XE6 machine at SNIC-PDC is not designed for these simulations. A restart of simulations every 24h is needed, and even if it is done automatically, each time, a part of the previous run is lost and there is a time delay between two successive jobs, so that it is effectively much longer to run a simulation on this machine.

Project Acronym: NUWCLAY

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CINES

PRACE Enabling sites: CINECA

PRACE Execution site: CINECA

PRACE Architectures: SP6, PLX cluster

Start enabling: November 2011

Start production: June2012

Project status: In progress (3%)

Description of project:

The primary research focus of this project is to obtain better molecular scale understanding of the adsorption and transport phenomena in clay systems used as natural and engineered barriers in the processes' nuclear waste management with the help of classical molecular dynamics simulations. Two sets of clay systems are being simulated at the first stage of the project: illite (muscovite) and smectite (montmorillonite) and their interaction with various metal cations and organic molecules present in interfacial aqueous solutions. LAMMPS and NAMD codes are used for the simulations.

Types of work undertaken:

By now a series of model systems have been prepared for the production runs and these systems are already tested in smaller-scale simulations on other machines. Compilation and optimization of LAMMPS has been done on CINECA's hybrid GPU cluster PLX.

Difficulties encountered:

The PI had initial difficulties using the security certificates properly and accessing the CINECA production site using the GSISSHTerm Java applet. While they were solving them, the preparatory work and initial simulations were running using their DARI allocations on the CCRT Curie and CINES Jade machines. The PI was not particularly persistent in solving the login problems at CINECA, because their work was successfully continued at CCRT and CINES. However, during the month of May 2012, with the help of the support personnel at CINECA and CINES they have finally solved all the problems with access to the computational resources using various means, including the GSISSHTerm applet. The production simulations have been started at the beginning of June 2012 and they are expecting to use up all the allocated time by the end of the project. The only difficulty they are experiencing at the moment is the very long waiting times. The PIs are currently working at optimizing their job scripts for better correspondence between the allowed and requested resources for their jobs in order to minimize the queue waiting time.

Extra enabling was needed to convert project from the original SP6 architecture to PLX.

Project Acronym: Planck-LFI

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CSC

PRACE Enabling sites: CSC

PRACE Execution site: CSC

PRACE Architectures: Cray XT4/5

Start enabling: November 2011

Start production: December 2011

Project status: In progress (70%)

Description of project:

Planck is a satellite mission of the European Space Agency to map the structure of the cosmic microwave background in unprecedented detail. The cosmic microwave background is radiation from the Big Bang, and it shows us the structure of the early universe. This DECI project supports the Planck mission by running the most resource-intensive tasks related to the analysis chain of data from the Low Frequency Instrument (LFI).

The project is a follow-up of the DEISA Science Community Support Initiative project Planck. It is a large collaboration of European and American research groups. The number of users is over 20 and they use many different applications. They also transfer a lot of data between CSC and NERSC (USA).

Types of work undertaken:

The project was helped with three problems. First one of the applications (Madam) was profiled, and performance bottlenecks were identified. However, no good ways to optimise the code were found. Second the users were helped to port the Planck likelihood code on the Cray XT4/XT5 of CSC. It wasn‘t ported already during DEISA. The third problem was related to data transfers. The project needs high bandwidth data transfers between CSC and NERSC. During DEISA, transfers were made with the gtransfer tool using HLRB2 of LRZ as a transit site. After HLRB2 was decommissioned, a new transit site – SARA – was taken into use. Tranfers via SARA perform well in one direction, but in the opposite direction the performance is only a fraction of what it was during DEISA and what it should be. The work to resolve the problem is going on.

Difficulties encountered:

The problem related to CSC–NERSC data transfers waits a solution. Despite long and careful study, it is not yet known why the transfer is so bad in one direction.

Project Acronym: TanGrin

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CSC

PRACE Enabling sites: CSC

PRACE Execution site: EPCC

PRACE Architectures: Cray XE6

Start enabling: November 2011

Start production: January 2012

Project status: In progress (40%)

Description of project:

This project uses the Gromacs molecular dynamics simulation package to unravel how the conformation of the integrin-bound talin depends on its interactions with lipids in a membrane.

Types of work undertaken:

Users were helped with accessing the execution site: Setting up accounts and installing certificates.

Difficulties encountered:

Maximum queue lengths on HECToR (12 hours) have been frustrating for the group. EPCC have been looking at introducing queues with a longer time limit.

Project Acronym: VIRonSAMs

Source of Project: DECI-7 (2011-2012)

PRACE Home site: CSCS

PRACE Enabling sites: CINECA, CINES

PRACE Execution site: CINECA, CINES

PRACE Architectures: Westmere Cluster; Jade Nehalem

Start enabling: December2011

Start production: December 2011

Project status: In progress (30%)

Description of project:

The major goal of the VIRonSAMs project is to identify the most important processes contributing to virus inactivation at interfaces, and to develop a comprehensive concept of the virus and surface parameters that dictate inactivation behavior. The simulations will focus on a model system representative of one of the great challenges to public health, namely viral contamination of water resources.

Types of work undertaken:

The project required NAMD 2.8 a well-known code. There were no major difficulties in porting the code. The project was able to start right away.

Difficulties encountered: None

Project Acronym: EC4aPDEs-2

Source of Project: DECI-7 (2011-2012)

PRACE Home site: EPCC

PRACE Enabling sites: EPCC,CSC, HLRS, IDRIS

PRACE Execution site: BSC, CSC, HLRS, IDRIS

PRACE Architectures: IBM cluster, CRAY XT4/XT5, NEC Nehalem cluster, IBM BG/P

Start enabling: November 2011

Start production: To be started

Project status: 0%

Description of project:

The project aims to foster a network of European scientists who are researching advanced methods for solving partial differential equations (e.g. finite element method, the extended finite element method, meshfree methods and molecular dynamics), set up a Virtual Laboratory for materials characterisation and to carry out benchmarking and performance optimisation in preparation for a future Tier 0 proposal.

Types of work undertaken: Setting up of accounts and installing certificates.

Difficulties encountered: PI has been held up due to input images being unavailable.

Project Acronym: HELIXKINETICS

Source of Project: DECI-7 (2011-2012)

PRACE Home site: EPCC

PRACE Enabling sites: EPCC, FZJ, ICHEC

PRACE Execution site: FZJ, ICHEC

PRACE Architectures: Intel cluster, SGI cluster

Start enabling: November 2011

Start production: November 2011

Project status: In progress (4%)

Description of project:

This project aims to test the validity of the theoretical models of helix-coil equilibrium and kinetics and determine optimal parameters for such models and to analyse experimental data directly, without needing to invoke a phenomenological model and to investigate whether simulations can explain the differences between the results of different experimental measurements.

Types of work undertaken: Telcon with PI was held. Setting up of accounts and installing certificates was done.

Difficulties encountered: None.

Project Acronym: HIFLY

Source of Project: DECI-7 (2011-2012)

PRACE Home site: EPCC

PRACE Enabling sites: EPCC

PRACE Execution site: EPCC

PRACE Architectures: Cray XE6

Start enabling: November 2011

Start production: November 2011

Project status: In progress (61%)

Description of project:

The aim of this project is the direct numerical simulation of flows occurring in insect and bio-inspired micro-air-vehicle flight.

Types of work undertaken: Visiting PI. Setting up of accounts and installing certificates.

Difficulties encountered:

The project was moved to the Cray XE6 system at EPCC after a long waiting for the original assigned system at PSNC which was not ready at the beginning of DECI7.

Project Acronym: HYDROGEN-Ils

Source of Project: DECI-7 (2011-2012)

PRACE Home site: EPCC

PRACE Enabling sites: EPCC, PDC

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: November 2011

Start production: November 2011

Project status: In progress (16%)

Description of project:

This project aims at a microscopic-level understanding of a Ru-catalyzed reaction affording the production of H2 from formic acid in ionic liquids, which is of prime interest in the framework of sustainable energy supply. High-level molecular dynamics simulations will allow the team to explain the key solvation effects occurring in this system and will provide detailed mechanistic information. The results will be of fundamental interest for the understanding of chemical reactivity in ionic solvents and will also be beneficial to experimentalists for optimizing catalytic systems.

Types of work undertaken: Work performed to help compile CPMD.

Difficulties encountered: None.

Project Acronym: HIGHQ2FF

Source of Project: DECI-7 (2011-2012)

PRACE Home site: FZJ

PRACE Enabling sites: SNIC-PDC

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: November 2011

Start production: June 2012

Project status: In progress (18%)

Description of project:

The nucleon, the hadronic state which makes up most of the observable mass in the universe, has been extensively studied both theoretically as well as experimentally. The internal structure of hadrons is studied by measuring form factors and generalized parton distributions, which can be associated to the charge and magnetization distributions as well as the

momentum distribution of quarks and gluons. Recently there have been many studies of these fundamental quantities using state-of-the-art simulations of Quantum Chromodynamics (QCD), the theory of the strong interactions. However, these calculations have been almost entirely restricted to momentum transfers (Q2) up to about 2 GeV2. This is due to the fact that one takes numerically the Fourier transform, which for large momenta becomes very noisy making calculations of the form factors at higher momentum transfers prohibitively expensive.

Types of work undertaken:

No enabling help was requested, accounts were created on the system

Difficulties encountered: None

Project Acronym: NR-NSNS-BHNS

Source of Project: DECI-7 (2011-2012)

PRACE Home site: FZJ

PRACE Enabling sites: CSC

PRACE Execution site: CSC

PRACE Architectures: Cray XT5

Start enabling: November 2012

Start production: January 2012

Project status: In progress (85%)

Description of project:

The goal of this project is to compute gravitational waves (GWs) from the inspiral and collision of binaries involving neutron stars in Einstein's theory of General Relativity (GR). Recently it has become possible to simulate several inspiral orbits and the merger and post-merger phase of compact binaries using the methods of Numerical Relativity (NR) on high performance parallel computers.

These simulations are of interest for the theoretical and technical challenges they represent but more importantly for their use in the larger context of GW detection. In support of the emerging field of GW astronomy, the PIs intend to compute highly accurate waveforms to investigate specific aspects of the most relevant astrophysical sources. The scientific objective of this proposal is to characterize the GW emission from the quasi-circular inspiral and merger of two binary systems

- mixed binary (black hole-neutron star) systems,

- unequal-mass binary neutron stars.

Types of work undertaken:

No enabling help was requested, only accounts were created on the system.

Difficulties encountered: None

Project Acronym: DIAVIB

Source of Project: DECI-7 (2011-2012)

PRACE Home site: HLRS

PRACE Enabling sites: CINECA, SARA

PRACE Execution site: CINECA, SARA

PRACE Architectures: IBM Power 6

Start enabling: November 2011

Start production: February 2012

Project status: In progress (41%)

Description of project:

Low dimensional semiconductor systems exhibit several favourable properties that are not present in their bulk counterpart, e.g. the optical gap of nanocrystals can be tuned with the characteristic size, however in many cases the size and composition is not exactly known. Recent developments allow the size- and shape-selected preparation of small diamond nanocrystals (diamondoids). These small diamond-like carbon cages can be considered as building blocks of larger nanodiamonds that have been extensively applied in biological studies where the optical properties are of crucial importance. It was found that optical gaps tended to be consequently larger in calculations than the measured ones. Since C-C and C-H bonds have strong vibration modes a strong electron-phonon coupling may shift the onset of absorption significantly that may explain the discrepancy between the experimental and simulation data. By taking into account the electron-phonon interaction, it will be possible to calculate the temperature dependent absorption spectrum close to the optical gap of small nanodiamonds by a parameter-free BSE method. These calculations would reveal how the absorption peaks can shift and broaden as function of the temperature where the spectra were recorded.

Types of work undertaken:

Accounts and administrative data were prepared by HLRS. Because the SP6 at CINECA has been decommissioned in May of this year SARA agreed to accept the transfer of the remaining budget from CINECA to the SARA account for the project DIAVIB. The PI asked for some assistance in porting the code to Huygens machine at SARA but he didn't provide any specifics about the kind of assistance he needs up until now. SARA pointed the PI in the direction of the local documentation on how to use Huygens.

Difficulties encountered:

The investigators had some delay to start production because of unforeseen problems with their program.

Because of a planned shutdown for replacement by a new machine the system at CINECA could be used till end of May only.

These two issues caused some additional administrative overhead.

Project Acronym: PHOTMAT

Source of Project: DECI-7 (2011-2012)

PRACE Home site: HLRS

PRACE Enabling sites: CINES, PSNC, HLRS

PRACE Execution site: CINES, PSNC

PRACE Architectures: Clusters

Start enabling: November 2011

Start production: December 2011

Project status: In progress (49%)

Description of project:

The project involves the design of fullerene and M- dithiolene-based materials, where M=Ni, Pd, etc, for photonic applications. The key parameters for such a design are the nonlinear optical (NLO) properties. The increasing demand for faster data processing, storage and distribution can only be fulfilled by ongoing miniaturisation of the basic electronic devices. Photonic technology, where light is used as information carrier instead of electrons, is considered to offer the answer. Thus, the basic concept on which the project is based, involves the design of novel derivatives for photonic applications, employing fullerenes and metal-dithiolenes as the main building blocks and the solution of several methodological problems.

The technical innovation potential is connected with the materials proposed to be designed and which are expected to have exceptionally large nonlinearities. Such materials are greatly needed by the photonic industry.

Types of work undertaken:

Accounts and administrative data were prepared by HLRS. The enabling of the software required proper and binary-efficient compilation of the third party application NWCHEM. This was done at PSNC. The system environment was tuned for specific needs. User level scripts were rewritten.

Difficulties encountered:

Because of unforeseen technical problems the investigators had serious difficulties to get their programs running at PSNC.

This required a serious amount of additional efforts by HLRS to discuss the problems and find solutions. The project was moved to the cluster architecture instead of SMP SGI, as originally allocated at PSNC. With PSNC agreement, the project has been granted the cluster access until March 2013.

Project Acronym: LGICTAMD

Source of Project: DECI-7 (2011-2012)

PRACE Home site: ICHEC

PRACE Enabling sites: ICHEC

PRACE Execution site: ICHEC

PRACE Architectures: X86 Cluster

Start enabling: December 2011

Start production: December 2011

Project status: In progress (20%)

Description of project:

This project aims to characterise the mechanisms of channel opening/closure with full atomistic Molecular Dynamics simulations. To overcome sampling limitations due to the large time scale of the process, the recently developed Temperature Accelerated Molecular Dynamics (TAMD) is to be used to efficiently explore the multi-dimensional conformational space of the receptor. Results will give an insight into the transmission of the conformational changes from the binding pocket in the extra-membrane domain to the trans-membrane domain. A detailed description of the mechanism governing opening/closure will also allow the identification of mechanisms governing the binding of different ligands to receptors.

Types of work undertaken:

Some parallel work was undertaken to explore the potential for GPUs to be used to address similar problems in the future. Minimal enabling work was also performed. Four user accounts (ssh + password) accessing Stokes via the UCD network were created.

Difficulties encountered: None

Project Acronym: NANOBIO-2

Source of Project: DECI-7 (2011-2012)

PRACE Home site: ICHEC

PRACE Enabling sites: ICHEC

PRACE Execution site: HLRS CINES

PRACE Architectures: X86 Clusters

Start enabling: January2012

Start production: May2012

Project status: In progress (46%)

Description of project:

This project proposes to study interfaces of biological systems with nanomaterials. In particular, the detailed mechanisms of protein and dye binding and adsorption to metal and metal oxide surfaces raise interesting and unresolved questions which only fully dynamic, electronic simulations by *ab initio* molecular dynamics methods can answer at the present time.

Types of work undertaken:

Setup x509v3 SSH to Laki at HLRS from Stokes at ICHEC was done. Setup GSI-SSH to Jade at CINES from Stokes at ICHEC via PRACE door node at SARA was done.

Difficulties encountered:

Project required building a patched OpenSSH client to enable access.

Delays getting grid cert for PI were encountered. Project required doing all grid cert security setup for PI.

Project Acronym: PICKH

Source of Project: DECI-7 (2011-2012)

PRACE Home site: IDRIS

PRACE Enabling sites: IDRIS, CINECA

PRACE Execution site: CINECA

PRACE Architectures: IBM SP6, IBM PLX

Start enabling: January 2012

Start production: March 2012

Project status: In progress (17%)

Description of project:

Production runs in 2D-3V configuration for a major cross-scale problem in space plasma research to better understand Sun-Earth interactions.

Types of work undertaken:

The PI has visited us at IDRIS in January. Different parallelization problems especially due to optimizations in the SP6 were solved when visiting CINECA. The PI had some problems consulting the DART using UBUNTU (version Java 1.5), he solved that using an MS Windows session. The code now runs on BG/P (Babel). One of the problems was the lack of compatibility with existing HDF5 libraries for writing outputs and restarts. This problem is solved; the code now uses the HDF5 version.

The PI has conducted a weak scaling study of the code. It is important to note that the algorithm requires global communications. The presented scaling is performed under the conditions of production runs of the project for which he thinks will use 2048 cores, with multi-threading. The decrease of performance is only ~ 15%.

Difficulties encountered:

Lack of compatibility with existing HDF5 libraries, as mentioned in the proposal was an obstacle.

The user has been informed that the IBM SP6 stopped at the end of May. IDRIS can't assign him a budget on Babel (BG/P), since not enough resources are available on the machine. The PI has been informed. He will wait until the CINECA BG/Q is available and make use of the IBM PLX cluster at CINECA.

Project Acronym: WESF

Source of Project: DECI-7 (2011-2012)

PRACE Home site: IDRIS

PRACE Enabling sites: IDRIS

PRACE Execution site: CSC, RZG

PRACE Architectures: Cray XT4/XT5, IBM BG/P

Start enabling: January 2012

Start production: July 2012

Project status: In progress (14%)

Description of project:

CFD simulations of practical gas turbine combustors.

Types of work undertaken:

The settings for chemistry codes were prepared.

Difficulties encountered: None

Project Acronym: CASiMIR

Source of Project: DECI-7 (2011-2012)

PRACE Home site: LRZ

PRACE Enabling sites: SARA

PRACE Execution site: SARA

PRACE Architectures: IBM Power 6

Start enabling: April 2012

Start production: May 2012

Project status: In progress (37%)

Description of project:

The project "Chemistry of the Atmosphere Simulated with an Earth System Model for the Interpretation of Satellite based Remote sensing observations (CASiMIR)" aims at an improved understanding of the physical and chemical processes, which determine the chemical state of the Earth's atmosphere. Particular regions of interest are the polar upper troposphere and stratosphere. Here, the occurrence of polar stratospheric clouds (PSCs) and the heterogeneous chemistry (e.g., chlorine activation) on their particle surfaces are important processes responsible for the spring-time ozone depletion (Antarctic ozone-hole). Despite their importance, these processes are still not understood in detail. New data from satellite based remote sensing instruments promise additional insight in comparison to simulations with state-of-the-art atmospheric chemistry models, which represent the current knowledge about the underlying processes. A direct comparison of observations from satellite with results from model simulations, in particular of short-term and (in time and space) highly variable phenomena, such as PSCs, is, however, not straightforward. The ECHAM/MESSy Atmospheric Chemistry (EMAC) general circulation model has therefore been equipped with a new diagnostic capability: For instruments on sun-synchronous orbiters, the highest possible model data coverage, suitable for point-to-point comparison between satellite observations and model results, is achieved at the lowest possible output storage requirements. This new technique is applied in a series of EMAC model simulations for process studies revealing and assessing the gaps in the current understanding of the chemistry and dynamics in the polar upper troposphere and stratosphere. The simulations include sensitivity studies on the PSC forming process and a simulation with a finer model grid-resolution to optimally represent the horizontal gradients of short-lived, highly variable constituents. The results of the analyses will feed back to the further model development. The project, as a detailed process study with a model of high complexity, is ambitious in terms of computational requirements and in particular in terms of data intensity, pushing the usage of resources, which are only available in a computational grid like PRACE, to the limits.

Types of work undertaken:

Creating accounts, providing additional storage space was done.

The meaning of PRACE_HOME, PRACE_DATA and PRACE_SCRATCH environment variables was explained to the PI and we assisted the home site in solving a problem with disk quota on the above-mentioned filesystems.

The PI did not have sufficient disc space on PRACE_DATA. SARA pointed the home site (LRZ) to RZG who hosts the PRACE_DATA filesystem of LRZ.

The usage of GRID software for transferring data from execution site to local storage was advised.

Difficulties encountered: None

Project Acronym: SIMONA

Source of Project: DECI-7 (20011-2012)

PRACE Home site: PSNC

PRACE Enabling sites: PSNC, SARA

PRACE Execution site: IDRIS, PSNC, SARA

PRACE Architectures: IBM Power6, IBM BG/P, SGI UV1000

Start enabling: March 2012

Start production: March 2012 (at SARA),

Project status: In progress (52%)

Description of project:

The simulations planned in the SIMONA project address the quantum phenomenological models which are the most reliable theoretical representatives of the physical molecular-based nanomagnets investigated recently and their reliability from the fundamental microscopic point of view assessed by the well established first-principle electronic structure calculations.

Exploiting a number of deterministic verified techniques (exact diagonalization, quantum transfer matrix, density-matrix renormalization group), the model calculations will be performed without any uncontrolled approximations and will be numerically accurate.

Types of work undertaken:

PSNC set up the user accounts in LDAP and helped PIs with obtaining grid certificates.

SARA solved a problem with investigators of the SIMONA project having trouble accessing Huygens. These problems were caused by wrong entries in the LDAP at PSNC. PSNC is helping with the compilation and tuning of the third party CP2K application on a new AMD architecture.

Difficulties encountered: There was a project move to the cluster architecture of PSNC, instead of SMP SGI allocated initially. Under PSNC agreement, the project has been granted the cluster access till March 2013.

Project Acronym: ARTHUS-3

Source of Project: DECI-7 (2011-2012)

PRACE Home site: RZG

PRACE Enabling sites: RZG

PRACE Execution site: FZJ

PRACE Architectures: Intel Nehalem@2.93

Start enabling: November 2011

Start production: December 2011

Project status: In progress (80%)

Description of project:

In this project the PI takes part in the competition for the currently most advanced simulations of the supernova evolution of massive stars and treats the neutrino-matter interactions in the supernova core with unprecedented accuracy. They plan to move towards three-dimensional models of core collapse supernovae with detailed neutrino-transport, supplemented by faster two-dimensional simulations to explore variations in parameter space.

Types of work undertaken:

RZG setup the account and gave assistance in using the target machine at FZJ. The code used in the ARTUS-3 project as a follow-up project of Arthus-2 project was expected to have already been optimized and ported to this architecture.

Tests, however, revealed that the performance of a new implementation of parallel HDF5 was not satisfactory, since for writing of the output only a bandwitdh of about 200 MB/s was achieved.

RZG assisted in removing the bottleneck by improving the parallel writing performance. As a result, the performance was improved by a factor of 5 with a bandwidth of about 1 GB/s. A new set of timing routines was introduced and the performance of the code was measured. With the help of this information, it was possible to further optimize some critical routines and to obtain a better scalability.

Difficulties encountered:

It turned out, that a new implementation of parallel HDF5 showed performance bottlenecks which had to be analyzed and measures had to be taken for improvements.

Project Acronym: EUTERPE-4

Source of Project: DECI-7 (2011-2012)

PRACE Home site: RZG

PRACE Enabling sites: RZG

PRACE Execution site: FZJ

PRACE Architectures: Intel Nehalem@2.93

Start enabling: November 2011

Start production: December 2011

Project status: Completed (100%)

Description of project:

First global gyrokinetic electromagnetic instability simulation in three dimensions.

Types of work undertaken:

This project is a successor of a previous project with the same code. This code was already ported and optimized for the target architecture. RZG therefore set up the accounts for seven investigators and helped the users to access the target site by getting and working with keys and certificates.

Difficulties encountered:

The PI was not able to access the resource consumption information given in the DART due to keystore problems.

Project Acronym: LASIPROD

Source of Project: DECI-7 (2011-2012)

PRACE Home site: RZG

PRACE Enabling sites: RZG

PRACE Execution site: LRZ

PRACE Architectures: Intel Westmere EX@2.4

Start enabling: November 2011

Start production: February 2012

Project status: In progress (6%)

Description of project:

Within LASiPROD, large scale molecular simulations of protein-DNA recognition in the combinatorial control of transcription are performed using the MD simulation packages NAMD and AMBER.

Types of work undertaken:

In preparation for the production runs, preparatory NAMD and AMBER installations and runs were performed initially on computers of the home site (RZG). In addition the remote visualization cluster was used to establish the basic visualization workflows and to demonstrate the suitability of the envisaged software tools. This allowed for a smooth transition to the execution site at LRZ.

Difficulties encountered: None

Project Acronym: SMARC

Source of Project: DECI-7 (2011-2012)

PRACE Home site: RZG

PRACE Enabling sites: RZG

PRACE Execution site: LRZ

PRACE Architectures: Intel Westmere EX@2.4

Start enabling: March2012

Start production: May 2012

Project status: In progress (2%)

Description of project:

The project runs new numerical experiments which will allow the study of the structure and evolution of an active region in the solar corona.

Types of work undertaken:

Project enabling included account provisioning, help with certificates and advice about the target execution system. Exchange of relevant information between home and execution sitewas also needed.

Difficulties encountered: None

Project Acronym: HRPIPE

Source of Project: DECI-7 (2011-2012)

PRACE Home site: SARA

PRACE Enabling sites: SARA, SNIC-PDC

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: November 2011

Start production: January 2012

Project status: Completed (100%)

Description of project:

The goal of the present research is to develop a highly accurate numerical model that is able to simulate, by means of DNS, turbulent pipe flow with Reynolds numbers in the range of the experiments carried out by (McKeon et al. 2004) and (Morrison et al. 2004).

Types of work undertaken:

SARA did a site visit to the PI and discussed several issues there:

- the setup of the PRACE infrastructure,
- the types of access possible
- preliminary work plan

SARA created a PRACE login for the PI. Furthermore SARA assisted the PI in clearing site specific issues to gain access to Lindgren, the Cray XE6 machine at SNIC-PDC.

SNIC-PDC activated the accounts on Lindgren and assisted PI with some job crash issues due to the memory overload.

Difficulties encountered: None

Project Acronym: RBflow-2

Source of Project: DECI-7 (2011-2012)

PRACE Home site: SARA

PRACE Enabling sites: SARA

PRACE Execution site: RZG, SARA

PRACE Architectures: IBM Power6

Start enabling: November 2011

Start production: February 2012

Project status: In progress (44%)

Description of project:

The goal of this project is to study the influence of the temperature boundary conditions at the sidewall on the heat transport in Rayleigh-Bénard (RB) convection - the buoyancy driven flow of a fluid heated from below and cooled from above. As the information on the entire flow field is known it is possible to see whether changes in the heat transport are reflected in the flow dynamics. It is emphasized that the Ra number regime in which the coexistence of different turbulent states is observed can only be achieved on state of the art computers and the simulations proposed here will break the current world record for high Ra number simulations.

Types of work undertaken:

This project continues the work that was done in the DEISA DECI project RBflow. So the PI is familiar with the PRACE infrastructure and the DECI procedures. Therefore SARA decided against a site visit and only had some phone and e-mail conversations with the PI, to prepare the project and to agree on a provisional work plan.

SARA created several PRACE logins for this project.

SARA advised the PI on how to use the PRACE module environment (the PI was still used to the DEISA environment), SARA increased his disc quota and his job quota for this project to obtain a higher throughput for the project.

Difficulties encountered: None

Project Acronym: DisMuN

Source of Project: DECI-7 (2011-2012)

PRACE Home site: SNIC-PDC

PRACE Enabling sites: SNIC-PDC, SARA

PRACE Execution site: SARA, SNIC-PDC

PRACE Architectures: IBM Power6, Cray XE6

Start enabling: November 2011

Start production: November 2011(at SNIC-PDC), March 2012 (at SARA)

Project status: In progress (38%)

Description of project:

This project is aimed at investigating the diffusion processes and spectroscopic properties of multicomponent nitrides using the most fundamental quantum mechanical equations of physics. Since the mixed systems form disordered solid solutions when grown as thin films the stochastic distribution of e.g. Ti and Al atoms in the crystals must be carefully considered which adds a huge complexity and computational challenge to this project. To investigate atomic diffusion in these materials electronic structure codes are used to calculate the energy barriers needed to be overcome by diffusing species, both inside bulk materials and on top of crystal surfaces. The different local chemical environments in the solid solutions will be studied using a large number of parallel calculations of different paths inside, and on top of, alloy supercells. In order to accurately interpret experimental spectroscopical measurements of nanostructured multicomponent nitrides a state-of-the-art modelling scheme will be applied for these properties: the Bethe-Salpeter equation. In this methodology the intricate quantum mechanics of the spectroscopical process is modelled far more accurately than with standard density functional theory methods. Using a clever parallel procedure these difficult equations will be solved to give a solid ground in the understanding of the nanostructure of multicomponent nitrides in collaboration with experimental work.

Types of work undertaken:

During the PRACE Tier-1 Training Workshop in Amsterdam (29 – 30 November 2011) SARA had a hands-on session with the PI of DiSMuN in which SARA assisted the PI in compiling his code "Exciting" on SARA's IBM Power6 machine, Huygens. SARA also provided the PI with some tips on which compiler flags to use for optimizing his code. Accounts were also created by SNIC-PDC and the project started its production runs on Cray XE6 machine, Lindgren.

Difficulties encountered: One of the codes needed engaged enabling work; however PI didn't provide the code to be worked on.

Project Acronym: MUSIC

Source of Project: DECI-7 (2011-2012)

PRACE Home site: SNIC-PDC

PRACE Enabling sites: IDRIS, PDC

PRACE Execution site: IDRIS

PRACE Architectures: IBM BG/P

Start enabling: January 2012

Start production: July2012

Project status: In progress (2%)

Description of project:

MUSIC (http://software.incf.org/software/music) is an API specification that allows for run-time exchange of data between parallel applications in a cluster environment. A pilot implementation was released 2009. MUSIC is designed specifically for interconnecting large-scale neuronal network simulators, either with each other or with other tools. In this project, MUSIC will be benchmarked and test its scalability up to hundreds of thousands of cores.

The primary objective of MUSIC is to support multi-simulations where each participating application itself is a parallel simulator with the capacity to produce and/or consume massive amounts of data.

Types of work undertaken:

Adaption was done to the MPMD mode on BG/P.

Difficulties encountered:

One of the users is Russian, the opening of an account for users that are not citizen of a European Union country requires the authorization of the CNRS Defense Officer. The user sent us all the forms and the account has been created.

Another problem is that the code is a MPMD application and is using the DCMF communication layer on BG/P. That implies a non-portability issue in future for other machines such as the IBM BG/Q.

IBM does not support MPI_COMM_SPAWN and MPI_COMM_SPAWN_MULTIPLE as the dynamic management of MPI processes is not implemented. That why is the only way to do MPMD program running is by executing two different codes within one MPI_COMM_WORLD. IDRIS also had a problem with the environment variable passed to each program: it has the same name but takes different values. The user had to change this in his application, it works only if the name of the environment variable is different for each code.

The MPMD runs well in SMP mode: the two codes are in a same big MPI_COMM_WORLD which IDRIS split in two sub-communicators, one sub-communicator per application. The SMP mode assumes there are the same number of processes in each sub-communicator; it is not the case in DUAL or VN mode.

Project Acronym: SIVE-2

Source of Project: DECI-7 (2011-2012)

PRACE Home site: SNIC-PDC

PRACE Enabling sites: SNIC-PDC, EPCC

PRACE Execution site: EPCC

PRACE Architectures: Cray XE6

Start enabling: November 2011

Start production: November 2011

Project status: In progress (67%)

Description of project:

The group has been developing high-performance simulation methods to analyse membrane fusion and are now extending these simulations to generate high-fidelity models of fusion in an experimental model systems, and predict the catalytic mechanism of influenza fusion proteins, particularly planning to examine how influenza-catalysed fusion is similar to or differs from protein-free fusion.

Types of work undertaken:

Setting up accounts and installing certificates.

Difficulties encountered: None

Project Acronym: SPIESM

Source of Project: DECI-7 (20011-2012)

PRACE Home site: SNIC-PDC

PRACE Enabling sites: SNIC-PDC

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: November 2011

Start production: November 2011

Project status: In progress (35%)

Description of project:

This project contributes to the "Reducing Uncertainty in global Climate Simulations using a Seamless climate prediction system (RUCSS)" project funded by the Spanish Science and Investigation Ministry. In RUCSS the aim is the testing the seamless approach (Palmer et al., 2008) for climate modelling with the EC-Earth Earth System Model (ESM) to constrain the sources of uncertainty in both short-term climate prediction and climate-change projections by increasing the understanding of the climate system. In this project, detailed analysis of climate simulations with different time horizons will be carried out using similar metrics to better understand the development of the systematic errors in EC-Earth with the hope of reducing the risk of overconfidence in both climate predictions and long-term projections. Among the processes that will be investigated are the water vapour feedback in the extratropics, the climate variability at the surface of the tropical Pacific and the extraordinary summer warming and drying observed and foreseen over Southern Europe.

Types of work undertaken:

Accounts created, requested software installed.

Difficulties encountered: There were some difficulties with the installation of auto submit tool that is specific for this code, however SNIC-PDC successfully managed to install it.

3.1 DECI7 applications support experience summary

As mentioned above DECI7 was a pilot call and served as a transitional stage between the DEISA and PRACE projects. Due to this transfer most of the projects had minor start-up delays. However these delays didn't cause major inconvenience to PIs to start their production runs.

Only four out of 35 projects didn't start their production runs. The PIs of three of these projects are simply not responsive despite multiple requests and efforts from home sites to help them start the production. These projects have been given a strict deadline to start their production runs and show a continuous character of usage. If this condition is not met, these three projects will be subtracted from the call and the CPU hours will be redistributed either to other DECI7 projects that have already spent the assigned CPU time and are eager to continue their runs or will be transferred to the projects from the DECI8 call.

The fourth project is progressing in accordance with their time plan and has a small amount of allocation which will be spent towards the end of the allocation period.

Generally the progress of the projects is going according to plan.

The six DECI7 projects that have requested more elaborate help with support are: SPIESM, DiSMuN, MUSIC, ElmerIce, Planck-LFI and PICKH.

- SPIESM project

The work with the SPIESM project was concentrated on the installation of specific software on the execution platform. The software being of a unique nature caused some problems, however through close collaboration with PI the problems were solved and the software installed.

- DiSMuN project

DiSMuN project required optimization and scalability work on one of the two codes they were planning to use. However the PI changed his decision and the code was never used in the runs and was not provided to PRACE experts. Thus despite the request no major support work was done for this project.

- MUSIC project

There was elaborative support work performed for the MUSIC project. The MPMD mode on BG/P system needed to be adapted. The code is an MPMD application and uses the DCMF communication layer on BG/P. That implies a non-portability issue in future for other machines such as the IBM BG/Q. IBM does not support MPI_COMM_SPAWN and MPI_COMM_SPAWN_MULTIPLE as the dynamic management of MPI processes is not implemented. That is why the only way to do MPMD program running is to execute 2 different codes within one MPI_COMM_WORLD. There was also a problem with the environment variable passed to each program: it has the same name but takes different values. The user is currently changing this in his application as it works only if the name of the environment variable is different for each codes.

- ElmerIce project

The main issue in connection with a compilation of ElmerIce on the Cray is that Compute Node Linux by default does not support shared objects. ElmerIce, on the other side, has a modular structure and hence depends on shared objects. Additionally, the main parallel sparse matrix solver libraries, Hypre and MUMPS (itself dependent on ScaLapack and BLACS) have to be compiled with particle independent code (using the -fPIC flag in common compiler

suites). The other important task completed was the optimisation of algorithms for discrete saddle point systems in Elmer. The Elmer/Ice applications bring along the fact that the Stokes equations have to be solved in connection with a strong non-linear power law rheology (Norton–Hoff law, Glen's flow law in glaciology). With the preconditioners traditionally available (basically ILU), in most real geometries it was very difficult, if not impossible, to achieve convergence of the linear system with memory and cycle-effective iterative Krylov subspace methods. The only available parallel direct solution method, MUMPS, on the other hand is memory intensive and limited in its scalability. In fact, it would have been better suited to a machine with more memory per core than the Cray. The research group is currently conducting benchmark runs on the Cray to elaborate the different numerical parameters and solution strategies of the subproblems in order to optimise the performance with the constraint of the robustness.

- Planck-LFI project

The Planck-LFI project was helped with three problems. First one of the applications (Madam) was profiled, and performance bottlenecks were identified. However, no good ways to optimise the code were found. Second the users were helped to port the Planck likelihood code on the Cray XT4/XT5. The third problem was related to data transfers. The project needs high bandwidth data transfers. During DEISA, transfers were made with the gtransfer tool using HLRB2 of LRZ as a transit site. After HLRB2 was decommissioned, a new transit site - SARA - was taken into use. Tranfers via SARA perform well in one direction, but in the opposite direction the performance is only a fraction of what it was during DEISA and what it should be. The work to resolve the problem is ongoing.

- PICKH project

PICKH had different parallelization problems especially due to optimizations on the SP6 system. These were solved with the help of the execution site. The code now runs on both PLX and BG/P systems and one of the problems on BG/P was the lack of compatibility with existing HDF5 libraries for writing outputs and restarts. This problem has also been solved and the code now uses the HDF5 version. The PI has conducted a weak scaling study of the code. It is important to note that the algorithm requires global communications. The presented scaling is performed under the conditions of production runs of the project for which he thinks using 2048 cores, with multi-threading. The decrease of performance is only ~ 15%).

Overall, there were no insurmountable difficulties reported during the application support work; the difficulties that were reported required some extra effort but in the end were solved. However, there were several points that didn't have direct connection to the application support task but were still successfully handled. These were for example the delays of the accounts due to the non-EU nationalities of the PIs and the EU country regulations, or the difficulties encountered at the execution sites that were new to the DECI infrastructure and thus required more time to adapt their systems to the PRACE common environment. Another difficulty that was noted was connected with one of the projects that requested no more than 256 cores for execution for runs longer than 200 hours. This project was assigned to a capability system which was incompatible for this project. In fact this project shouldn't have been classified as Tier-1 project.

4 Enabling Work on DECI8 Projects

The DECI8 call was combined together with the 4th PRACE call for applications. It was launched on the 2nd of November 2011 and closed on 10th of January 2012. The access and thus application support for DECI8 accepted projects started from 1st of May 2012.

Out of 49 projects, 35 DECI8 proposals have been accepted of which about 5 requested essential support of between 3 to 6 months of work for enabling of these codes. The list of this projects as well as the requested support is listed in Table 4.

Home site	Project	Execution site(s)	Enabling PMs
BSC	CIO2_deg	CINES, UYBHM	0,5
BSC	FULLDRUG	EPCC	1,0
CINECA	LBglaSS	CINECA	0,5
CINECA	NAHUJ	CINECA, WCSS	3 to 6
CINECA	OPTOCHIMEMD	CSCS, SARA	0,5
CINECA	WFNUC	CSCS, RZG	0,5
CINES	SMARTWING	ICHEC, WCSS	0,5
CSC	CYTODYN	SNIC-PDC	0,5
CSC	PARAMETER	EPCC	0,5
CSC	Photoreception	FZJ, HLRS, LRZ, RZG	0,5
CSCS	DrugEffluxMechanism	IDRIS	1,0
EPCC	CONTRAR	SNIC-PDC	0,5
EPCC	POLARIZABLEFOLDBIND	SNIC-PDC	0,5
EPCC	TLRSim	CSCS	0,5
HLRS	POEMatCASP	CINES	0,5
ICHEC	RCR2CP	SNIC-PDC	1,0
ICHEC	SARCEMS	ICHEC	0,5
ICHEC	TiO2-Interface	UYBHM	0,5
IDRIS	CoMoPro	RZG	1,0

IDRIS	MOLED	CSC, ICHEC	1 to 3
IDRIS	VIPforVPH	EPCC	1 to 3
LRZ	FFF	CINECA	0,5
PSNC	ELORBIC	SARA	1 to 3
PSNC	MLMJTAX	UYBHM	1,0
PSNC	NELC	EPCC	1,0
RZG	EUTERPE-5	FZJ	0,5
RZG	LASIPROD-2	SNIC-PDC, IDRIS	0,5
SARA	NanoTherm	EPCC, SARA	1,0
SARA	TRANSPART	SNIC-PDC	0,5
SNIC-LUNARC	PLANETESIM	FZJ, RZG, ICHEC	5,0
SNIC-PDC	CANONS	CSCS	0,5
SNIC-PDC	MBIOMARK	CSCS	0,5
SNIC-PDC	PIPETURB	EPCC, CSC	0,5

Table 4: Enabling effort requests of DECI8projects with home and execution sites

Table 5 lists the same DECI8 projects per architecture.

Architecture	**DECI8 Projects**
IBM BG/P	CoMoPro, DrugEffluxMechanism, LASIPROD-2, WFNUC
IBM Power 6	ELORBIC, OPTOCHIMEMD, PLANETESIM, NanoTherm
CRAY (XT4/5, XE6)	CANONS, CONTRAR, CYTODYN, FULLDRUG, LASIPROD-2, MBIOMARK, MOLED, NanoTherm, NELC, OPTOCHIMEMD, PARAMETER, PIPETURB, POLARIZABLEFOLDBIND, RCR2CP, TLRSim, TRANSPART, VIPforVPH,WFNUC
Clusters (SuperMUC migration, Bull Nehalem, NEC Nehalem, SGI ICE E8200, SGI UV1000, HP)	EUTERPE-5, FFF, LBglaSS, MLMJTAX, MOLED, NAHUJ, Photoreception, PLANETESIM, POEMatCASP, SARCEMS, SMARTWING, TiO2-Interface

Table 5: DECI8 projects per architecture

Table 6 lists the DECI8 projects per discipline.

Discipline	DECI8 Projects
Astro Sciences	PLANETESIM
Bio Sciences	CIO2_deg, CYTODYN, DrugEffluxMechanism, FULLDRUG, LASIPROD-2, MLMJTAX, OPTOCHIMEMD, Photoreception, POEMatCASP, POLARIZABLEFOLDBIND, SARCEMS, TLRSim, VIPforVPH
Earth Sciences	PARAMETER, RCR2CP
Engineering	FFF, LBglaSS, NAHUJ, PIPETURB, SMARTWING, TRANSPART
Materials Science	CANONS, CoMoPro, CONTRAR, ELORBIC, MBIOMARK, MLMJTAX, MOLED, NanoTherm, NELC, TiO2-Interface
Informatics	MOLED
Plasma & Particle Physics	EUTERPE-5, WFNUC

Table 6: DECI8 projects per discipline

Below is the detailed list of the application support work for each DECI8 project. The project status indicates the amount of CPU hours used in relation to the granted amount of CPU hours expressed in percentage.

Project Acronym: CIO2_deg

Source of Project: DECI8 (2012-2013)

PRACE Home site: BSC

PRACE Enabling sites: BSC

PRACE Execution site: CINES, UYBHM

PRACE Architectures: Intel Nehalem@2.93, Intel Harpertown@3

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

The project chlorite degradation by chlorite dismutase enzymes is led by Pietro Vidossich. The objective is to determine the reaction mechanism of reaction 1 ($ClO_2^- \rightarrow Cl^- + O_2$) as catalyzed by Chlorite dismutase and pinpoint the structural motifs at the origin of the enzyme striking specificity. To this scope, they will use *ab initio* (Car-Parrinello) and classical molecular dynamics simulations to determine the free energy profile of reaction 1 as well as of ligand binding and intermediate(s) dissociation. The codes used are CPMD and NAMD.

Types of work undertaken:

BSC have created the LDAP accounts and contacted both CINES and UYBHM local supports to check the creation of the accounts. The users were trained to the use the infrastructure.
Difficulties encountered:

PIs encountered some problem with the certificate creation process that were fixed with BSC support. The PI delayed the production runs until July 1st.

Project Acronym: FULLDRUG

Source of Project: DECI8 (2012-2013)

PRACE Home site: BSC

PRACE Enabling sites: BSC

PRACE Execution site: EPCC

PRACE Architectures: HeCToR XE6

Start enabling: May 2012

Start production: May 2012

Project status: In progress (40%)

Description of project:

Accurate calculation of drug binding thermodynamics and kinetics led by Dr. Francesco Luigi Gervasio.

They will apply Molecular dynamics simulations to study the association of drugs and drug-like molecules to two classes of very flexible and pharmaceutically important anticancer targets, namely the Abl and Src tyrosine kinases and the heat shock protein 90. They state-of-the-art simulations will be fully validated by micro-calorimetry, surface-plasmon resonance experiments and NMR. The experimentally validated results will provide a solid basis for the understanding of subtle biophysical effects in molecular association and guidance for the systematic improvement of the target and drug force-fields, when needed. They will use Gromacs.

Types of work undertaken:

LDAP accounts were created and local EPCC support was contacted. Setting up accounts and installing certificates.

Difficulties encountered: None

Project Acronym: LbglaSS

Source of Project: DECI-8 (2012-2013)

PRACE Home site: CINECA

PRACE Enabling sites: CINECA

PRACE Execution site: CINECA

PRACE Architectures: Westmere GPU cluster

Start enabling: May 2012

Start production: May 2012

Project status: In progress (2%)

Description of project:

Among a variety of numerical methods for complex flows, both atomistic and macroscopic, mesoscopic lattice Boltzmann (LB) models have recently been developed, which prove capable of reproducing a number of qualitative features of soft-flowing materials, such as slow relaxation, dynamical heterogeneities, aging and others. The PIs have developed a multi-GPU CUDA implementation of this extended LB model which provides very significant time gains with respect to the previous, albeit highly-tuned, CPU implementation. The expected outcome of the numerical experiments PIs would like to run within the PRACE initiative is a better understanding of the complex flow properties of foams and real emulsions, from mesoscale up to their hydrodynamical behaviour and rheological properties. In particular, the idea is to improve LB models to describe emulsions and their properties under confinement in different geometries while changing the boundary conditions.

Types of work undertaken:

Account were created by CINECA. The PI and team were already familiar with the PLX artchitecture at CINECA.
Difficulties encountered: None.

Project Acronym: NAHUJ

Source of Project: DECI-8 (2012-2013)

PRACE Home site: CINECA

PRACE Enabling sites: CINECA, WCSS

PRACE Execution site: CINECA, WCSS

PRACE Architectures: Intel Westmere/GPU cluster, Cluster

Start enabling: May 2012 (at CINECA), June2012 (at WCSS)

Start production: To be started

Project status: 0%

Description of project:

The aim of this work is the study of the fluid dynamic behavior of underexpanded hydrogen jets by using a High Performance Computing (HPC) methodology. The analysis will be carried out by employing a two-dimensional axial symmetric in-house code which is able to take into account real gas effects by employing either Van der Waals or Redlich-Kwong equations of state (EoS). The first aim of this project is to evaluate the influence of real gas effects on hydrogen jets structure. In fact, very recent works have shown the importance to employ real gas equations dealing with highly underexpanded hydrogen jets. A parametric analysis will be carried out by varying the injection pressure and temperature, in order to investigate the features of underexpanded jets and real gas effects under different conditions
Types of work undertaken: Account creation at CINECA. WCSS is gathering information about the project's own codes.

Difficulties encountered:

The project is still in enabling. The project has requested particular enabling effort in the porting of the code for the GPU. WCSS still doesn't have access to the CINECA LDAP to get the user accounts data. This is in progress.

Project Acronym: OPTOCHIMEMD

Source of Project: DECI-8 (2012-2013)

PRACE Home site: CINECA

PRACE Enabling sites: CINECA, CSCS, SARA

PRACE Execution site: CSCS, SARA

PRACE Architectures: Cray XE6, IBM Power6

Start enabling: May 2012

Start production: July 2012

Project status: In progress (8%)

Description of project:

Optogenetics is a very recent technique in cell biology which involves the use of genetically encoded, light-gated proteins to perturb and control cellular and organismal behavior in a spatiotemporally precise fashion. A remarkable application is the modulation of cellular signalling as for example the control of gene transcription and expression. This can be obtained by engineering chimeric proteins where the light-switched domain is properly fused to a protein involved in the transcription process. To realize these chimeras experimentally, atomic detailed knowledge of the protein's structure, relevant interactions, and conformational characteristics is strongly needed. In this project, recent computational techniques will be applied and further developed to efficiently explore the Free Energy landscape describing the conformational properties of engineered light-switched chimeric proteins. Results will provide high-resolution information to guide the experimental realization of the chimeras.
Types of work undertaken: Accounts were created.

Difficulties encountered:

The project is still in enabling. The PIs have problems in obtaining X.509 certificates which are required for accessing the resources at SARA (their institution does not have a recognised Registration Authority).

Project Acronym: WFNUC

Source of Project: DECI-8 (2012-2013)

PRACE Home site: CINECA

PRACE Enabling sites: CINECA, CSCS, RZG

PRACE Execution site: CSCS, RZG

PRACE Architectures: CRAY XE6, BG/P

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

Atomic nuclei, hadrons and various high density systems, like e.g. neutron stars and QCD matter at extreme conditions, are systems governed by the strong interaction. The nature of QCD, which governs the interactions between quark and gluons confined in hadrons, is such that there is a residual interaction between nucleons, known as strong interaction. The aim of

the project is the description of various phenomena involving nucleons and nuclei by using realistic wave functions of few- and many-body systems.

Types of work undertaken: Accounts were created.

Difficulties encountered: None.

Project Acronym: SMARTWING

Source of Project: DECI8 (2012-2013)

PRACE Home site: CINES

PRACE Enabling sites: WCSS

PRACE Execution site: WCSS

PRACE Architectures: Cluster XEON X5650@2.67

Start enabling: June 2012

Start production: To be started

Project status: 0%

Description of project:

This project concerns the analysis by numerical simulations of compressible flows or flows with variable density around aerofoils in 2D or 3D. PIs aim to better understand the physical mechanisms related to the instabilities and the unsteadiness arising and the transition in flows around obstacles since the very first steps towards turbulence at moderate Reynolds numbers in order to better model these mechanisms at high Reynolds number.

Types of work undertaken: CINES has helped PIs with obtaining certificates, set up the LDAP accounts and checked the readiness of the execution machine at WCSS. Users were helped with accessing the execution site. WCSS is gathering information about the NSMB codes, including contacts with the PIs on specific requirements. The application environment has been prepared.

Difficulties encountered: None.

Project Acronym: CYTODYN

Source of Project: DECI-8 (2012-2013)

PRACE Home site: CSC

PRACE Enabling sites: CSC

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: May 2012

Start production: In progress

Project status: In progress (16%)

Description of project:

This project uses the NAMD molecular dynamics simulation package to study the cyt bc1 complex in explicit lipid bilayer at physiological salt concentration. The main task of this

study will be the calculatation of the free energy of substrate binding and to elucidate substrate bonding modes.

Types of work undertaken: Users were helped with accessing the execution site.

Difficulties encountered: None.

Project Acronym: PARAMETER

Source of Project: DECI-8 (2012-2013)

PRACE Home site: CSC

PRACE Enabling sites: CSC

PRACE Execution site: EPCC

PRACE Architectures: Cray XE6

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

This project aims to apply advanced parameter estimation techniques to quantify the uncertainty of a numerical weather prediction model, and to tune the predictive skill of it by means of algorithmic model parameter estimation. The model under study is Echam5.

Types of work undertaken: Users were helped with accessing the execution site, setting up accounts and installing certificates.

Difficulties encountered: None.

Project Acronym: Photoreception

Source of Project: DECI-8 (2012-2013)

PRACE Home site: CSC (external)

PRACE Enabling sites: CSC, HLRS, FZJ, LRZ, RZG

PRACE Execution site: HLRS, FZJ, LRZ, RZG

PRACE Architectures: Clusters with Intel Xeon processors

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

This project uses the Firefly quantum chemistry package to study light-induced protein dynamics, in order to provide new insight in the molecular basis of vision.

Types of work undertaken:

Users were helped with accessing the execution sites and porting their application.

Difficulties encountered: None.

Project Acronym: DrugEffluxMechanism

Source of Project: DECI-8 (2012-2013)

PRACE Home site: CSCS

PRACE Enabling sites: IDRIS

PRACE Execution site: IDRIS

PRACE Architectures: IBM BG/P

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

As with many membrane transport proteins, the function of P-gp relies on three elementary mechanisms: selectivity, permeation and gating. Using molecular dynamics simulations, this study aims at identifying the key molecular interactions that sustain these basic functions. Simulations of both the P-gp and Sav1866 proteins embedded in a lipid membrane shall be performed.

How the proteins interact with its lipid environment is not clear, e.g. the number of lipids potentially occupying the cavity is unknown. The first stage of this project will thus involve a series of test simulations to identify the optimal lipid configurations. Next, the focus will be placed on the mechanism allowing the substrates to move from the lipid membrane to the core of the transporters.

Types of work undertaken:

The project required NAMD 2.9 a well-known code. There were no major difficulties in porting the code. The project was able to start right away

Difficulties encountered:

As of today, there were no technical difficulties in preparing this project. However, because the student involved in this project is Chinese, the project might be delayed up to three months before IDRIS obtains the authorization to open an account for the student.

Project Acronym: CONTRAR

Source of Project: DECI8 (2012-2013)

PRACE Home site: EPCC

PRACE Enabling sites: EPCC, SNIC-PDC

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

This project investiges a redox- and conformation-based molecular switch. The project investiges a recently synthesized molecule with two charge centres that is capable of storing up to two electrons. The mechanisms by which the different charge and conformational states are stabilized, which in return can provide an avenue to localize and control the transfer of single electrons at a scale of around 1 nm is investigated.

Type of work undertaken: Information provided to PI about getting accounts.

Difficulties encountered: No response from PI yet.

Project Acronym: POLARIZABLEFOLDBIND

Source of Project: DECI8 (2012-2013)

PRACE Home site: EPCC

PRACE Enabling sites: EPCC, SNIC-PDC

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: May 2012

Start production: May2012

Project status: In progress (3%)

Description of project:

The group intend to use a state of the art, polarizable force field to address the specific aim of using all-atom molecular dynamics simulations to determine the atomic-resolution mechanism of coupled protein folding and nucleic acid binding. Specifically, they will simulate coupled folding and binding between the Jun-Fos heterodimer and DNA.6. Jun and Fos are components of the transcription factor AP1, which regulates gene expression in response to stimuli.

Types of work undertaken: Setting up accounts and installing certificates was done.

Difficulties encountered: None

Project Acronym: TLRSim

Source of Project: DECI8 (2012-2013)

PRACE Home site: EPCC

PRACE Enabling sites: EPCC, CSCS

PRACE Execution site: CSCS

PRACE Architectures: Cray XE6

Start enabling: May 2012

Start production: May 2012

Project status: In progress (48%)

Description of project:

This project uses a simulation approach to probe the molecular determinants of TLR4 ligand recognition and activation, towards the development of novel therapeutic treatments.

Explicitly-solvated, all-atom molecular dynamics simulations will be performed for the entire signalling-competent receptor complex in the presence of a range of bound ligands, with typical systems amounting to approximately half a million atoms. Long-timescale trajectories will provide a means to systematically probe the dynamic effects of a ligand library on receptor stability.

Types of work undertaken: Setting up accounts and installing certificates was done.

Difficulties encountered: Dealing with some problems accessing disk space.

Project Acronym: POEMatCASP

Source of Project: DECI8 (2012-2013)

PRACE Home site: HLRS

PRACE Enabling sites: CINES, HLRS

PRACE Execution site: CINES

PRACE Architectures: Clusters

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

Proteins are the nanoscale machines of all cellular life. Most proteins fold into a unique three-dimensional structure, determined entirely by their amino acid sequence, in a slow and complicated process that is still not fully understood. Because sequencing techniques are far more efficient than structure resolution, predicting the structure of proteins and their functional complexes is one of the major challenges in the life sciences. Closely related is the investigation of protein-protein interactions as one of the most important mechanism of signaling in biological systems.

After the complete genome of many species has been sequenced, there is a huge gap between the number of known sequences and the number of known structures. Computational methods for protein structure prediction are increasingly used to close this gap, but progress for proteins with low sequence similarity to structure the resolved proteins has been slow.

The PIs have developed a biophysics-based atomistic simulation techniques for protein folding and protein structure prediction. Application of this methodology often has direct applications in the life-sciences: These techniques have been applied in close cooperation with experimental groups to elucidate the genetic origin of some human developmental disorders and also apply them to design inhibitors for protein-protein interactions.

In this project these methods have been combined with homology modelling techniques and efficient methods for model generation to predict the structure of larger proteins.

Types of work undertaken: Accounts and administrative data were prepared by HLRS.

Difficulties encountered:

Two of the six investigators are not citizens of the European Union. Because of the legal situation in France additional efforts are required to allow access for these two to the system at CINES.

Project Acronym: RCR2CP

Source of Project: DECI-8 (2012-2013)

PRACE Home site: ICHEC

PRACE Enabling sites: ICHEC

PRACE Execution site: SNIC-PDC

PRACE Architectures: CRAY XE6

Start enabling: June 2012

Start production: To be started

Project status: 0%

Description of project:

The aim of this project will be to use the output of the most up to date European Global Climate Model, EC-Earth and dynamically downscale the data through the use of a Regional Climate Model to a scale more useful to local planning (i.e. water resource and flood defences). A key limitation of Global Climate Models (GCM's) is the fairly coarse horizontal resolution, typically 3.75o by 2.5o (500 km x 300 km). For practical planning, countries require information on a much smaller scale than GCM's are able to provide. One of the solutions is to embed a Regional Climate Model (RCM) in the GCM.

Types of work undertaken: Setup of GSSAPI SSH to Lindgren at SNIC-PDC from Stokes was done. Investigating queue setup and job submission for PI was needed. Dr. Adam Ralph of ICHEC collaborates with the PI on project.

Difficulties encountered: Building a patched OpenSSH client to enable access was required.

Project Acronym: SARCEMS

Source of Project: DECI-8 (2012-2013)

PRACE Home site: ICHEC

PRACE Enabling sites: ICHEC

PRACE Execution site: ICHEC

PRACE Architectures: X86 Cluster

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

This project is about an advanced computational framework that will capture the response of cells to dynamic loading being developed by considering two mutually dependent cellular processes; i.e. the formation of contractile stress fibres in response to mechanical and chemical stimuli and the formation of traction dependent on focal adhesions. Model development will include 3D implementation of a constitutive formulation that predicts the distribution and contractility of stress fibres. This implementation will be used to predict the behaviour of cells subjected to static loading such as micropipette aspiration and parallel plate compression. A thermodynamically motivated model for focal adhesion formation will be

used in tandem with this stress fibre formulation to predict the static response of cells spread on different elastic substrates.

Types of work undertaken:

Minimal enabling work for home site was required: One user account (ssh + password) accessing Stokes at ICHEC via NUIG network was needed. ABAQUS is already available.

Difficulties encountered: None

Project Acronym: TiO2-interface

Source of Project: DECI-8 (2012-2013)

PRACE Home site: ICHEC

PRACE Enabling sites: ICHEC

PRACE Execution site: UYBHM

PRACE Architectures: X86 Cluster

Start enabling: June 2012

Start production: To be started

Project status: 0%

Description of project:

This project proposes to study interfaces of biological systems. The TiO2-Interfaces project will undertake first principles density functional theory (DFT) simulations of technologically important interfaces between the two dominant polymorphs of titanium dioxide (TiO2), namely anatase and rutile. This is a key materials system in photocatalysis, which has the potential to be an extremely important technology for energy generation and depollution, using only sunlight and cheap, widely available materials in the process.

Types of work undertaken: Setup GSI-SSH to Karadeniz at UHEM from Stokes via the PRACE door node at SARA was done. ICHEC tested the connection with the account of Eoin McHugh (ICHEC).

Difficulties encountered: PI is having difficulty getting grid certificate in order to access the system.

Project Acronym: CoMoPro

Source of Project: DECI-8 (2012-2013)

PRACE Home site: IDRIS

PRACE Enabling sites: IDRIS

PRACE Execution site: RZG

PRACE Architectures: IBM BG/P

Start enabling: June 2012

Start production: To be started

Project status: 0%

Description of project:

Collective Motions in Protein Crystals

Types of work undertaken:

The PI visited IDRIS in July. IDRIS contacted the PI in order to create the PRACE accounts, explained certificates and PRACE infrastructure (DART, TTS, and training session in the PATC).

Difficulties encountered: None.

Project Acronym: MOLED

Source of Project: DECI-8 (2012-2013)

PRACE Home site: IDRIS

PRACE Enabling sites: IDRIS, ICHEC, CSC

PRACE Execution site: CSC, ICHEC

PRACE Architectures: Cray XT4/XT5, SGI Altix ICE 8200EX

Start enabling: June 2012

Start production: To be started

Project status: 0%

Description of project:

Multiscale Modelling of Organic LED

Types of work undertaken:

The PI visited IDRIS in May. In order to create the PRACE accounts, IDRIS explained certificates and PRACE infrastructure (DART, TTS, and training session in the PATC) to the PI. One of the users is interested in attending an OpenMP and MPI session (IDRIS sessions in June and September).

Difficulties encountered: Certificate problems, the Belgium users didn't have an adequate certificate, specifically a certificate in p12 format. The problem is solved now.

Project Acronym: VIPforVPH

Source of Project: DECI-8 (2012-2013)

PRACE Home site: IDRIS

PRACE Enabling sites: IDRIS, EPCC

PRACE Execution site: EPCC

PRACE Architectures: CRAY XE6

Start enabling: June2012

Start production: To be started

Project status: 0%

Description of project:

Virtual Imaging Platform of virtual physiological Human.

Types of work undertaken:

Contacted the PI in order to create the PRACE accounts, explained certificates and PRACE infrastructure (DART, TTS, training session in the PATC). Set up accounts and installed certificates.

Difficulties encountered:

One of the users is Colombian, the opening of an account for users that are not citizens of a European Union country requires the authorization of the CNRS Defense Officer. The user sent IDRIS all the forms and the account has been created.

Project Acronym: FFF

Source of Project: DECI8 (2012-2013)

PRACE Home site: LRZ

PRACE Enabling sites: CINECA

PRACE Execution site: CINECA

PRACE Architectures: (GPU) Cluster

Start enabling: May2012

Start production: To be started

Project status: 0%

Description of project:

The aim of the project is the development of efficient, reliable and future-proof numerical schemes and software for the parallel solution of partial differential equations (PDEs) arising in industrial and scientific applications. The interest is in technical flows including Fluid-Structure interaction, chemical reaction and multiphase flow behaviour which can be found in a wide variety of (multi-)physics problems. In this approach, both numerical and hardware efficiency are addressed simultaneously: On the one hand, the transition of today's computational hardware towards parallel (and heterogeneous) architectures is in progress and therefore all levels of parallelism (vectorisation, parallelism on the core level in multi- and many-core CPUs and accelerator devices like GPUs and finally on the node level within distributed memory clusters) have to be exploited. Algorithms and whole solvers have to be tailored with respect to the target hardware in order to achieve a significant amount of the parallel peak performance. On the other hand, the sole concentration on hardware efficiency does not carry out the whole job (and in some cases may be counter-productive): Numerical efficiency plays a crucial role and itself includes multiple levels that can be optimised. Starting with the overall numerical and algorithmic approach required for the solution of a given domain specific problem (i.e. discretisation of the governing equations in time and space), stabilisation, linearisation of non-linear problems and finally the solution of the linear problems and smoothing therein, all these aspects together with the aforementioned levels of parallelism bear a large amount of interdependencies. In the proposed project, PIs want to improve the parallel numerical software framework FEATFLOW (www.featflow.de) and augment this powerful simulation toolkit for academic and industrial usage. The planned improvements take both aspects of efficiency into account in order to make it ready for future HPC-architectures: Novel numerical- and physics-components as well as software-techniques for massively parallel (heterogeneous) compute resources are going to be employed that extend the applicability of the package to current and future real-world problems in the field of CFD.

Types of work undertaken: Accounts were created

Difficulties encountered: None

Project Acronym: ELORBIC

Source of Project: DECI-8 (2012-2013)

PRACE Home site: PSNC

PRACE Enabling sites: PSNC

PRACE Execution site: SARA

PRACE Architectures: IBM Power 6

Start enabling: To be started

Start production: To be started

Project status: 0%

Description of project:

Molecular-based metallic clusters and chains behave like individual quantum nanomagnets, displaying quantum phenomena on a macroscopic scale. In view of potential applications of such materials in magnetic storage devices or in envisaged quantum computer processors as well as in the low-temperature refrigerants, the accurate simulation of these complex objects becomes the key issue. The magneto-structural correlations, the role and mechanism of magnetic anisotropy and intrinsic quantum effects following from the geometrical frustration induced by the topological arrangement of spins or particular interactions count among the new challenges for computer simulations. The simulations planned in the SINA project address the quantum phenomenological models which are the most reliable theoretical representatives of the physical molecular-based nanomagnets investigated recently and their reliability from the fundamental microscopic point of view assessed by the well established first-principle electronic structure calculations.

Types of work undertaken: The project has not yet started.

Difficulties encountered: None

Project Acronym: MLMJTAX

Source of Project: DECI-8 (2012-2013)

PRACE Home site: PSNC

PRACE Enabling sites: PSNC

PRACE Execution site: UYBHM

PRACE Architectures: Cluster Intel Nehalem@2.93

Start enabling: To be started

Start production: To be started

Project status: 0%

Description of project:

Microtubule stabilizing agents (MSA) interfere with disassembly of microtubules in rapidly dividing cancer cells. Paclitaxel (Taxol®), the complex, diterpenoid natural product and the effective MSA, binds to tubulin in a stoichiometric ratio and operates by blocking

microtubule dissociation into tubulin dimers and finally causes apoptosis i.e. programmed cell death. Although the EC structure of paclitaxel on tubulin Zn+2 sheets showed the location of the ligand, the conformation of paclitaxel molecule was not determined with sufficient precision. The estimation of the bioactive conformation indicated two structures: the so-called T-taxol, proposed by Emory University, Atlanta, GA group and PTX-NY referred to the New York Sony Brook group. In the present project computational project questions are addressed in order to estimate the conformational space (PES) of paclitaxel as well to judge these two proposals of molecular shape. Another purpose of the present work is to precisely determine the possible hydrogen bond patterns, including cooperative enhancement, and to illuminate the weakly recognized aromatic and olefinic fragments orbital interactions because such information is important to better understand the nature of non-bonding interactions and their effect on final internal energy. Since density functional methods fail to accurately describe weak π-π interactions, the use of second order Møller-Plesset (MP2) or coupled cluster CCSD(T) (SP) is predicted at cc-pVDZ and aug-cc-pVDZ basis set. The stacking bonding, due to London dispersion energy, will be additionally estimated to characterize attractive interaction energies of benzene-benzene and benzene-ethylene complexes of paclitaxel fragments. It is possible that the detailed knowledge on the paclitaxel binding site regarding its PES led to the development of second-generation taxanes.

Types of work undertaken:

The users are in the progress of obtaining personal certificates. The computations will start in July.

Difficulties encountered: None

Project Acronym: NELC

Source of Project: DECI8 (2012-2013)

PRACE Home site: PSNC

PRACE Enabling sites: PSNC, EPCC

PRACE Execution site: EPCC

PRACE Architectures: Cray XE6

Start enabling: May 2012

Start production: To be started

Project status: 0%

Description of project:

The goal of this project is a generation of well optimized ECG wave functions for a six-electron molecule (methylidynium, CH+) at the equilibrium distance. This cation is one of the first species discovered in the interstellar space and essential in the formation of carbon hydrates. The project aims to provide reliable data for solving questions pertaining to astrophysics and for understanding the role of CH in the interstellar chemistry. For that purpose, the PIs plan to employ the ECG method and the massive computations to a large scale deterministic optimization of the energy and wave function according to a well-defined strategy.

Types of work undertaken: Users were helped with obtaining certificates and accessing the execution site. Testing of the software on the PSNC local machines against the different compiler switches and timing results was performed.

Difficulties encountered: None

Project Acronym: EUTERPE-5

Source of Project: DECI-8 (2012-2013)

PRACE Home site: RZG

PRACE Enabling sites: RZG

PRACE Execution site: FZJ

PRACE Architectures: Intel Nehalem@2.93

Start enabling: June 2012

Start production: July 2012

Project status: In progress (9%)

Description of project:

Follow-up project of EUTERPE-4. The first global gyrokinetic electromagnetic instability simulation in three dimensions.

Types of work undertaken:

EUTERPE-5 has been mapped again on the JUROPA system at FZJ, so no further application enabling work is necessary for this project.

Difficulties encountered: None

Project Acronym: LASIPROD-2

Source of Project: DECI-8 (2012-2013)

PRACE Home site: RZG

PRACE Enabling sites: RZG

PRACE Execution site: IDRIS, SNIC-PDC

PRACE Architectures: BlueGene/P and Cray XE6

Start enabling: June 2012

Start production: To be started

Project status: 0%

Description of project:

Within LASiPROD, large scale molecular simulations of protein-DNA recognition in the combinatorial control of transcription are performed using the MD simulation packages NAMD and AMBER.

Types of work undertaken:

For LASIPROD-2 different execution sites have been selected, and the compute contingent was an even split between the BlueGene/P system Babel at IDRIS and the Cray XE6 system Lindgren at SNIC-PDC. The project enabling work for the new machines is in preparation.

Difficulties encountered: None

Project Acronym: NanoTherm

Source of Project: DECI8 (2012-2013)

PRACE Home site: SARA

PRACE Enabling sites: EPCC, SARA

PRACE Execution site: EPCC, SARA

PRACE Architectures: Cray XE6, IBM Power 6

Start enabling: May 2012

Start production: May 2012

Project status: In progress (5%)

Description of project:

On the one hand, a fundamental methodology has been developed for the first principles prediction of thermoelectric qualities of materials within density functional theory (led by M. Verstraete). On the other hand, the methodology will be applied to two important classes of materials (functional oxides, led by Ph. Ghosez ; and intermetallics, led by J.-Y. Raty) which appear to be the most promising candidates to address respectively high (600-700K) and room temperature (300-400K) thermoelectric applications.

Types of work undertaken:

Setting up user accounts and installing certificates was done. SARA introduced the PI to the PRACE infrastructure via e-mail. Because the PI was located in Belgium and because the e-mail conversation went very smoothly it was not deemed necessary to visit the PI on site.

SARA created several PRACE logins for this project.

On request from the PI SARA built and installed a special version of the Lapack library that is able to efficiently use some implementations of Lapack routines from the IBM ESSL library. This version is called CCI (Common Calling Interface for Lapack/ESSL). SARA also created a special module file for this Lapack implementation.

SARA is in discussion with the PI to also install the application code that is used by the project (ABINIT) for general use.

Difficulties encountered:

The application seems to be crashing sometimes (MPI tasks aborting), but the job that is governing the execution of the program doesn’t stop in this case. Although ultimately this should be handled by the application itself, SARA nevertheless suggested a procedure to cancel the job in the case where some MPI tasks within the job abort.

Project Acronym: TRANSPART

Source of Project: DECI-8 (20012-2013)

PRACE Home site: SARA

PRACE Enabling sites: SNIC-PDC, SARA

PRACE Execution site: SNIC-PDC

PRACE Architectures: Cray XE6

Start enabling: May 2012

Start production: July2012

Project status: In progress (1%)

Description of project:

In this project the flow case of a transitional spatially evolving boundary layer exposed to free-stream turbulence, as typically observed on turbine blades is studied. The study is focussed on the advection of small inertial particles in transitional intermittent flows. Such a computational study is based on highly resolved DNS.

Types of work undertaken:

SARA visited the PI on site to explain the PRACE infrastructure and procedures to the PI. Because the PI already had an approved DECI project within DEISA, the PI was already familiar with several aspects of the infrastructures and procedures. SARA created several PRACE logins for this project. SARA also explained the extra procedures on top of the standard PRACE requirements (grid certificate) that were necessary to obtain access to Lindgren.

SARA discussed the dataflow and planning of permanent storage of the project output.

Difficulties encountered: None

Project Acronym: PLANETESIM

Source of Project: DECI-8 (20012-2013)

PRACE Home site: SNIC-LUNARC

PRACE Enabling sites: SNIC-LUNARC, SNIC-CHALMERS

PRACE Execution site: FZJ, RZG, ICHEC

PRACE Architectures: Cluster, IBM Power 6

Start enabling: May 2012

Start production: June 2012

Project status: In progress (6%)

Description of project:

The aim of this research project is to use high-resolution computer simulations to understand the birth sizes of planetesimals. The size distribution of the planetesimals in the asteroid belt and Kuiper belt shows a break around 50 km in radius. Modelling planetesimal formation at much higher resolution than previously, using PRACE supercomputers, the project will investigate the size distribution of planetesimals down to 30 km in radius and compare to the observed size distributions of asteroids and Kuiper belt objects.

Types of work undertaken:

General enabling support such as assistance in applying for certificates and installing software required to securely access the PRACE production system was done. SNIC-LUNARC explained the PRACE research infrastructure and the resources available for the project to the PI.

The project asked for help to improve the I/O architecture of the simulation code and to deploy a better performing FFT-library. This work has started. SNIC-LUNARC and SNIC-Chalmers are currently analyzing the existing application code and working on proposals of how to implement the new features. Two face-to-face meetings involving the PI and PRACE staff have been held so far.

Difficulties encountered:

The Terenea certificates used by the researchers caused problems when accessing the IBM Power 6 system at RZG. An alternative way of secure access to the production system has been provided to the research group by RZG.

The PI of the project currently has problems accessing the trouble ticket system. These problems are still under active investigation. As a temporary work around, PRACE staff from the home site are entering problem reports into the trouble ticket system.

Project Acronym: CANONS

Source of Project: DECI8 (2012-2013)

PRACE Home site: SNIC-PDC

PRACE Enabling sites: SNIC-PDC, CSCS

PRACE Execution site: CSCS

PRACE Architectures: Cray XE6

Start enabling: May2012

Start production: To be started

Project status: 0%

Description of project:

For the modelling of the structural materials, special focus will be devoted to modelling the behaviour under irradiation of Oxide Dispersion Strengthened (ODS) steels. This new class of nano-structured materials has shown good resistance to radiation effects. However, these novel materials have not, and cannot, be tested in real life for timescales corresponding to the lifetime of a reactor. Therefore, it is proposed to model the ageing and degradation of the mechanical properties of the ODS steels and other nano-structured materials. The modelling will be based on existing experimental data and on first principles quantum mechanical calculations, feeding these data into higher scale models, such as kinetic Monte-Carlo, where the long term evolution of the alloy microstructure can be simulated. The most compute intensive part of this project consists of the first principles calculations. The ODS and nano-structured materials have been shown in many studies to have a very good response to neutron irradiation. Especially the irradiation induced swelling and creep are minimal. However, these studies have all been performed for short time spans where the nano-clusters have no time to disintegrate and diffuse into the matrix or to grain boundaries or other sinks. Therefore, it is of critical importance to evaluate what will happen over longer times. The stability, under irradiation, of these nano-clusters can be assessed using a multi-scale

modelling approach. The largest computational load of these two efforts will be to perform first principles calculations using the VASP code, which has been optimized on numerous architectures, including Cray XE6.

Types of work undertaken: Setting up accounts and installing certificates has been done.

Difficulties encountered: None

Project Acronym: MBIOMARK

Source of Project: DECI8 (2012-2013)

PRACE Home site: SNIC-PDC

PRACE Enabling sites: SNIC-PDC, CSCS

PRACE Execution site: CSCS

PRACE Architectures: Cray XE6

Start enabling: May2012

Start production: To be started

Project status: 0%

Description of project:

Alzheimer□s disease is one of the most prominent cause of the acquired dementia in elderly patients and it affects around 35.6 million people worldwide. In Sweden among the 160 thousand with dementia around 45% have been diagnosed with Alzheimer□s disease. Cases of Alzheimer□s disease have a profound impact on the patients and their families and the overall impact of this disease on the whole society is expected to increase in the future with an aging population in Europe. Early diagnostics of the Alzheimer□s disease is essential for efficient treatment of this disease and efficient screening of the people within risk groups. Unfortunately, currently options for clinical diagnostics of early stages of the Alzheimer□s disease is very limited and development of novel clinical imaging techniques are highly desirable. The present research project aims to address this problem and focuses on the development of the electron paramagnetic resonance imaging technique, which is a promising methodology for *in vivo* imaging of early damage to brain tissue cause by Alzheimer□s disease. Within this project PIs aim to develop novel fluorescent spin labels, which are employed as the contrast agents in the electron paramagnetic resonance imaging, using the state of the art molecular modeling tools.

Types of work undertaken: Setting up accounts and installing certificates has been done.

Difficulties encountered: None

Project Acronym: PIPETURB

Source of Project: DECI8 (2012-2013)

PRACE Home site: SNIC-PDC

PRACE Enabling sites: SNIC-PDC, EPCC

PRACE Execution site: EPCC

PRACE Architectures: Cray XE6

Start enabling: May2012

Start production: To be strated

Project status: 0%

Description of project:

The aim is to study fully developed high-Reynolds number turbulent pipe flow through direct numerical simulations (DNS). DNS attempts to resolve all relevant scales of the turbulent flow. These will be carried out using the massively parallel DNS code available at KTH Mechanics, nek5000, which is based on an accurate and efficient spectral-element discretization. Pipe flow is the case which is easiest to realise in experiments. However, due to numerical difficulties related to the cylindrical coordinates and the corresponding numerical singularity arising along the symmetry line, it is the only canonical flow case that has not yet been thoroughly studied using DNS, as opposed to plane channels and boundary layers.

Types of work undertaken: Setting up accounts and installing certificates has been done.

Difficulties encountered: None

4.1 DECI8 applications support experience summary

The access period for DECI8 projects started in May 2012 and thus only about two months have passed since writing this deliverable. All 35 projects have started and have already been ported and started their test runs. Some even managed to start production runs. The application support help requested by 5 projects has just started and no difficulties have been reported to this point. However the major part of the work on DECI8 projects is yet to come and more will be reported in the next deliverable of this task. It is worth noting that the start of DECI8 projects was on time and went very smoothly.

5 DECI9 call

The 5th PRACE call including DECI9 has been launched on 17th of April 2012 and was closed on May 30th 2012. 45 DECI9 proposals for Tier-1 access have been submitted. The proposals went through technical evaluation and currently are being distributed to scientific committees for scientific evaluations. The outcome of the scientific evaluations, and as a consequence the list of accepted projects and the estimate of application support work, will be known after August 2012 and thus will be reported in the upcoming final deliverable of this task in August 2013.

6 Summary and Future Work

During the first year of PRACE-2IP project, task T7.2 has successfully accomplished its planned work. Technical evaluations of three DECI calls 7, 8, and 9 were performed and access and application support was provided to 70 projects from DECI7 and DECI8. All these projects have successfully started either their production runs or start-up and enabling work. While projects of the DECI7 call are already in the middle of their production runs, most of the projects of DECI8 have just started their test runs. Experts from all engaged in the T7.2 task centres are helping the PIs with the questions arising during execution of the projects. Six DECI7 projects received significant help with application support in accordance with their requests. The work on another five DECI8 projects is in progress.

In the next deliverable the report on the progress of DECI8 projects as well as DECI9 accepted projects that will start their execution period from November 2012 for the duration of one year will be given. A detailed overview of application support work for the projects requesting more engagement of PRACE experts will be summarised as well.

Other interesting ongoing work is the creation of the web-based tool for DECI procedures such as technical and scientific evaluations. Even though T7.2 is not directly involved with the implementation activities of this tool, it still follows the process as a consultant in certain questions connected with the technical evaluation process. A short up-to-date report will be given on this activity as well.